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Uncertainty in North American Wet Deposition Isopleth Maps Effect of Site Selection and Valid Sample Criteria

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UNCERTAINTY IN NORTH AMERICAN WET DEPOSITION ISOPLETH MAPS: EFFECT OF SITE SELECTION AND VALID SAMPLE CRITERIA

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This report considers several issues related to the preparation of isopleth maps for the display of spatial patterns of wet deposition. The valid sample criteria and data completeness rating used in the data summarization process are described. The data interpolation technique, kriging, is presented and it's derivation in terms of generalized least squares regression is given. Four different annual summaries for pH, sulfate concentration, and sulfate deposition in 1986 are prepared using either the Unified Deposition Database Committee (UDDC) definition of valid sample criteria or a relaxed valid sample criteria and the UDDC data completeness rating or a relaxed data completeness rating. The kriged estimates for the different annual summaries and the differences between these estimates are contoured. The effects of relaxing the valid sample criteria and data completeness rating are discussed. Conclusions are drawn about network operation, network design and the uncertainty of contour maps. It is recommended that in the case where the objective is contour maps to show regional patterns, the emphasis in most regions needs to be on the number of valid samples per site and the regional representativeness of the sites.

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1.0 INTRODUCTION

Junge (1963) operated the first precipitation chemistry network in the United States and reported the data by using isopleth maps of ion concentrations. Since then a number of regional and national isopleth maps of precipitation chemistry data have been published: Semonin (1981), Cowling (1982), Calvert et al. (1983), Munger and Eisenreich (1983), Barrie and Hales (1984), Ellis et al. (1983), and Husar (1988). The researchers determined the location of the contours on these maps either by subjectively using expert opinion to hand draw them or simple weighting schemes such as inverse distance squared.

More recently several researchers have used the geostatistical technique termed kriging to estimate the spatial surface and then display the surface using isopleth maps. Eynon and Switzer (1983) and Finkelstein (1984) published isopleth maps based on two alternative kriging approaches. Since then a number of authors have used kriging in the production of maps: Seilkop and Finkelstein (1987), Barchet (1987), Wampler and Olsen (1987), Guertin et al. (1988), Haas et al. (1988), and Venkatram (1988). Bilonick (1985) and Le and Petkau (1988) applied spatial time series models to precipitation chemistry data in North America.

The National Atmospheric Deposition Program (NADP) and the Acid Deposition System (ADS) regularly publish United States and North American isopleth maps of annual precipitation chemistry. NADP coordinates the NADP/NTN network and uses the network data to produce annual maps starting with 1983 data. NADP (1987) is an example of their publications. The ADS combines the NADP/NTN network data with data from several other North American precipitation chemistry monitoring networks to produce annual isopleth maps for North America. See Olsen and Watson (1984), Olsen and Slavich (1985), Olsen and Slavich (1986), Sweeney and Olsen (1987), Sweeney and Olsen (1988), and Olsen (1988). NADP uses a constrained distance-squared weighting function to estimate the surface while ADS uses kriging to estimate the surface. A more detailed

explanation comparing the approaches is given in an informal report by Olsen (1988), which is reproduced as Appendix A.

In 1988, researchers concerned with wet deposition data organized two spatial analysis workshops. The first workshop on regional analysis of wet deposition for effects research was held June 7-8, 1988 in Corvallis, Oregon. Vong et al. (1989) summarize the workshop discussion. The workshop focussed on issues connected with estimating wet deposition an non-monitored sites and did not explicitly consider presentation of regional wet deposition surfaces as isopleth maps. One conclusion of the workshop is that kriging is currently a preferred technique for interpolation to non-monitored sites. The second workshop focussed explicitly on presentation as isopleth maps and was held October xx, 1988 in Champaign, Illinois. The workshop organizers prepared standard data sets for North America and invited six different organizations to use the standard data sets to produce isopleth maps. Methods used by the organizations included hand drawn by an expert, inverse distance squared, Cressman's objective weighting, other objective analysis schemes, and several kriging alternatives. No workshop report is available at this time. Our conclusions from the workshop are that regardless of the interpolation technique the broad overall regional features of the surface are very similar across techniques but local features do differ when different techniques are used.

The production of an isopleth map involves: 1) selection of sites to be used in surface estimation, 2) calculation of an annual summary value at a monitored site, 3) selection of a surface estimation technique, 4) selection on how to display the estimated surface, and 5) production of a final document quality display. Decisions made for each of these can affect the final display and how it is perceived. When the surface is displayed using isopleth maps, alternative choices can result in different maps. Even if agreement on these issues could be reached, the wet deposition data has measurement error associated with the sampling and laboratory analysis process. Hence an isopleth map has uncertainty associated with the location of its isopleth lines due to

measurement error and to the uncertainty associated with possible alternative production decisions.

Isopleth maps are a common method of summarizing and displaying the spatial pattern for wet deposition over North America. The process includes determining annual summaries at wet deposition monitoring sites, selecting sites with representative data, estimating a spatial surface by interpolating the selected sites to a regular grid, and then displaying the surface using an isopleth map. It is generally recognized that the location of the isopleth lines can be affected by the procedures used at each stage of the process. In fact, isopleth maps for the same annual time period and ion species constructed by different organizations have been constructed, for example, the pH map for 1985 given in the NAPAP Interim Assessment report (Barchet 1987) and the pH map for 1985 in the NADP/NTN Annual Data Summary report (NADP 1987). The maps do differ and the question arises as to why. (Olsen 1988). A natural follow-up question is can an agreement be reached on what the "correct" process is to go from sample data collected at sites to the "correct" isopleth map.

An isopleth map is a display of an estimated surface. Data at monitored sites used in the surface estimation process are only estimates of wet deposition at the monitored site. Hence, the location of the isopleth lines would still have uncertainty associated with them even if organizations would agree to use the same data, same sites and same surface estimation methodology. The uncertainty of the data at the site and the uncertainty associated with estimating wet deposition at non-monitoring locations as part of the surface estimation methodology both contribute to the uncertainty in the location of the isopleth lines. A natural question is how to determine (estimate) the uncertainty on the location of the isopleth lines.

This report investigates the impact on estimated surfaces due to the use of alternative procedures for estimating wet deposition at individual monitoring sites and for selecting representative monitoring sites. The impact of alternative surface estimation methodologies is not explicitly investigated.

2.0 DESCRIPTION OF WET DEPOSITION DATA SETS

The purposes of this section are: 1) to describe wet deposition monitoring data sources, data summarization processes, and site selection processes that have been used by organizations who produce isopleth maps for wet deposition ion species and 2) define alternative data sets used in this report. No attempt is made to include all procedures that have been used. The discussion is focussed on the processes used to define the alternative data sets used later in the report.

2.1 WET DEPOSITION DATA SOURCES

Various federal, state, and local governmental agencies and private industry organizations support networks of sites for the collection and chemical analysis of precipitation samples, i.e., for wet deposition monitoring. Determining which networks of sites to include is a primary decision in a study of wet deposition spatial patterns. Issues typically considered in the selection process are: 1) objectives and spatial coverage of the network, 2) quality assurance associated with the data, 3) compatibility of network monitoring, laboratory, and data validation protocols, 4) availability of data, and 5) special requirements/restrictions by spatial pattern study organization. The first three issues are associated with the representativeness and compatibility of the data. The latter two issues are typically operational issues rather than representativeness issues. The selection of different networks to be included in spatial pattern studies for the same year can potentially be a major source of differences between isopleth maps prepared by two organizations. Interpretation or comparison of isopleth maps requires an understanding and assessment of the network selection criteria used.

The wet deposition data used for this study are from six regional or national networks that contribute data to the Acid Deposition System (ADS) (Watson and Olsen 1984). The network's are the Multi-State Atmospheric Pollution and Power Production Study initiated precipitation chemistry network (MAP3S/PCN), the National Atmospheric Deposition

Program/National Trends Network (NADP/NTN), the Utility Acid Precipitation Study Program (UAPSP), the Canadian Acid Precipitation Monitoring Network (CAPMoN), the Acidic Precipitation in Ontario Study daily (APIOS-D) and cumulative (APIOS-C) networks. Sweeney and Olsen (1988) give additional descriptions of the networks. Criteria used in selecting these networks are: 1) the network provides regional or national coverage at regionally representative sites, 2) each network has an implemented quality assurance program, 3) the network chemical analysis laboratories participate in an inter-laboratory comparison program, and 4) the data are readily available in a common format from ADS.

The decision to use these networks does impact the spatial pattern displayed by an isopleth map. Site selection protocols for the networks restricts location of sites within urban areas and minimizes impact of local point source emissions. Although not an explicit site selection protocol, almost all sites are located away from mountainous regions. Consequently, isopleth maps based on the networks may not reflect variations in the spatial surface related to local point sources effects, urban influences, or elevation effects. Any spatial pattern derived will at best reflect the broad regional or national structure of wet deposition. The impact of this decision on isopleth maps will not be explicitly studied in the report.

The networks used in the study each has a chemical analysis laboratory that performs sample analyses and a data management function that checks the reasonableness of the sample analysis results using information available from the analysis and from the sample field notes. That is, each network receives data from a laboratory which has been subjected to internal laboratory checks and to sampling protocol checks. The checks result in supporting comments and data flags being attached to the samples. The ADS data base incorporates all of the comments, codes and flags. A quality assurance program is used by each of the networks to insure that their protocols are implemented and their laboratories are in control. In addition, all of the laboratories participate in interlaboratory comparison studies.

2.2 DATA SUMMARIZATION PROCESS

Calculation of an annual summary from sample data collected at a site requires criteria for assessing whether a sample data value is valid or invalid for the purposes of the study. These criteria are called valid sample criteria. Even with careful attention, some samples collected must be declared invalid because of the violation of some aspect of a network's protocol that affects the sample's representativeness of the precipitation chemistry. In some cases, such as severe contamination by debris, the sample is clearly not representative of the precipitation chemistry. In other cases, such as bulk sampling or non-protocol sample period, whether the sample is representative of the precipitation chemistry during the period is not as clear. Currently, a sample's representativeness and a criteria for a valid sample have not been generally developed and accepted. Valid sample criteria that do exist are based on the best professional judgements of wet deposition monitoring researchers.

To study the impact of different valid sample criteria, hence indirectly sample representativeness, two alternative valid sample criteria have been defined for the study. One alternative uses the valid sample criteria developed by the Unified Deposition Database Committee (UDDC) (Olsen et al 1987). The other alternative relaxes the UDDC valid sample criteria by removing two UDDC valid sample criteria. This alternative is termed the relaxed valid sample Criteria.

The UDDC valid sample criteria have been designed to incorporate each network's comments, codes and flags into the decision process of determining whether an individual wet deposition sample result is to be included or excluded from a summary. The discussion on screening for valid samples is stated in terms of the ADS data base common record format (Watson and Olsen, 1984) with some reference to network specific codes as necessary for clarification.

All networks include note codes which are informational in nature. Some codes denote reasons why sample results are not available or reported. Other codes describe conditions present in the field, and

during sample transit and sample receipt. Unless explicitly stated elsewhere, these note codes are not used in determining whether a sample is valid. The basic premise is that each network has screened individual sample results for possible contamination. If a sample result passes the network's screening, it is assumed that possible sample contamination indicated by field or lab comments did not materially affect the sample ion species concentrations.

A set of valid sample criteria has been designed for each network. Each sample associated with a sampling period is screened to determine whether the sample meets specific criteria. The screening criteria use the informational comments and codes provided by each network. The criteria are:

- All sampling periods for which it is known that no precipitation occurred are considered valid sample periods. This applies mainly to weekly, monthly and 28-day sampling protocols. For event and daily sampling protocols the absence of a sample record for a day implies that no precipitation occurred.

- The wet deposition sample must be a wet-only sample. All samples identified as bulk, partially bulk or undefined are invalid.

- Wet deposition samples that have insufficient precipitation to complete a chemical analysis for a specific ion species are invalid for that specific ion species. Event/daily samples are most likely to have this occur.

- An individual ion species concentration accompanied by a comment code designating the measurement to be "suspect" or "invalid" is declared an invalid sample. Deletion of the ion species concentration by the network for the same reason has the same result.

- The actual sampling period for a wet deposition sample must be close to the network's protocol sampling period. Specifically, the following conditions lead to an invalid sample:

  For NADP/NTN, actual sample period less than 6 days or greater than 8 days. This includes all NADP/NTN samples coded "LD" with measured precipitation.

  For APIOS-C, actual sample period less than 21 days or greater than 35 days.

  For UAPSP, actual sample period greater than 1 day.

The restriction to wet-only samples used for the UDDC valid sample criteria may be too stringent and their exclusion may result in a bias. For the networks used in the study, the sample chemistry is checked for internal consistency and for consistency with historical data from the site. Hence severe contamination due to an exposed bucket will cause other data flags to be set. Large differences between wet-only and bulk sample chemistry may not be common in networks designed with wet-only sampling protocols. Typically, the sampler fails at some time during the sampling period, violating the protocol. Exclusion of bulk samples can cause a bias in annual precipitation weighted mean concentrations, especially if an ion species has a seasonal pattern at a site. It may be more appropriate to include a bulk sample as the best estimate of concentration rather than exclude the sample and in effect use the annual precipitation weighted mean concentration as the estimate for the sample. No detailed study has been completed to study this question.

The UDDC valid sample criteria also restricts the actual sample period length of a sample to be within a few days of the network's protocol sampling period. For example, NADP/NTN samples must be 6, 7, or 8 days in length. The reason for the restriction is to maintain consistency within the data. Again however, no objective study has been

completed to show the effect of departure from a daily, weekly, or four-weekly sampling period. The criteria may be overly restrictive and introduce a bias as stated above for bulk samples.

2.3 SITE SELECTION PROCESS

Calculation of an annual summary based on valid data at a site does not imply that the annual summary represents the chemistry of precipitation that occurred at the site during the year. This may be due to the sampling not being completed continuously at the site, to incomplete collection of individual precipitation events (low collection efficiency), to chemical changes occurring in the sample during or after sample collection, or to precipitation associated with invalid samples having concentrations different than that associated with valid samples (e.g., seasonal effects).

The study defines and uses two alternative site selection criteria for assessing the completeness, i.e.,representativeness, of the annual summary. One is the UDDC data completeness criteria which incorporates both an annual and a quarterly criteria. The other, called the relaxed data completeness criteria, is a relaxed UDDC criteria which eliminates the UDDC quarterly criteria and weakens the UDDC annual criteria.

The Unified Deposition Database Committee defined five quantitative data completeness measures and assigned annual and quarterly thresholds to each of the five measures in constructing their UDDC data completeness criteria. The following questions concerning data completeness and temporal representativeness motivated the measures: for what portion of the summary period is the occurrence and amount of precipitation known; what portion of the precipitation volume collected is associated with valid deposition samples; what percent of the time and what percent of the samples collected are associated with valid samples; and what is the ratio of the wet deposition sample volume to the precipitation measured by a standard gage?

Data completeness measures are based on the assumption that the entire season or year consists of sample periods that account for every

day of the summary period. It is normal for a site to have incomplete information for some precipitation events during a summary period, to deviate from established collection protocols due to circumstances outside the operator's control, or to collect samples that are subsequently eliminated during the network's data screening process. Therefore, it is necessary to establish criteria for determining when sufficient valid wet deposition data are present to calculate a meaningful seasonal or annual summary for a site. Data completeness measures are designed to quantify the amount of information upon which a data summary is based and enable criteria to be established that indicate the quality of the summary. Five data completeness measures are proposed: percent precipitation coverage length, percent total precipitation, percent valid sample length, percent of samples with measured precipitation that are valid and percent collection efficiency. A sixth measure, percent sea salt correction is applied to sulfate summaries for sites within 100 km of a coast. Definitions for the data completeness measures are given in Table 2.1.

The data completeness measures are the basis for assigning a data completeness level (1 to 4) to each seasonal and annual summary. The criteria for the data completeness levels are given in Table 2.2. A summary with data completeness level 1 has the best information, or the highest level of data completeness. The least confidence is given to a summary with data completeness level 3. Level 4 summaries fail level 3 criteria. They are viewed as not providing a representative summary for the period. In order for a data summary to be assigned a specific level, all criteria listed for the level must be met. The most favorable level attained is assigned to the summary. A summary that does not meet one or more of the criteria for level 3 is assigned as level 4.

The collection efficiency data completeness level criteria for a seasonal summary is relaxed somewhat for Canadian winter summaries compared to other seasons due to the generally poorer collector performance for snow sampling. If the criteria for other seasons is applied to winter months when a large percentage of the precipitation in

Canada is in the form of snow, then only a few locations meet even the level 3 criterion. It is believed that a lower percentage could be accepted for winter because the problems are primarily due to undercatch of snow. An under-collected snow sample may reasonably represent the concentration but not the deposition.

The data completeness level for an annual summary is based on annual criteria as well as criteria for the four quarters, January-March, April-June, July-September, and October-December, which comprise the year. The addition of quarterly criteria to the annual criteria is to insure that adequate data from each quarter is present in the annual summary. Because the emphasis is on insuring adequate data for an annual summary, some quarterly criteria are relaxed from the seasonal criteria (see Table 2.2).

The relaxed data completeness criteria applies only the annual %PCL (≥90%) and %TP (≥60%) data completeness measures. All quarterly criteria are dropped. Sites meeting the relaxed data completeness criteria but not the UDDC criteria, almost exclusively fail the quarterly criteria. The quarterly criteria are intended to insure that all quarters of the year are represented in an annual summary. However, the criteria may be overly restrictive. The relaxed criteria result in almost all sites that monitored continuously during a year being included in the study.

TABLE 2.1. Definition of Data Completeness Measures

Data Completeness Measure	Definition
%PCL	Percent precipitation coverage length is the percent of the summary period for which information on whether or not precipitation occurred is available. If precipitation is known to have occurred during a particular sampling period but no measurement of the amount is available, then no knowledge of precipitation is assumed. This measure can be less than 100% because the site started (stopped) operation after (before) the beginning (end) of the summary period or because equipment or operator problems caused the site to be shut down for a portion of the summary period.
%TP	Percent total precipitation is the percent of the total precipitation depth measured that is associated with valid samples collected during the summary period.
%VSL	Percent valid sample length is the percent of the days durin the summary period for which valid samples are obtained. Note that sample periods with no precipitation are considere valid samples.
%VSMP	Percent valid samples with measured precipitation is the percent of all wet deposition samples during the summary period that are valid samples.
%COLEFF	Percent collection efficiency is the ratio of the wet deposition sample volume (converted to a depth) to the total precipitation depth as measured by a collocated rain gauge. Only valid samples with both a collocated standard rain gaug and sample volume measurement available are used.
%SEASALT	Percent sea salt correction is the percent of the average sulfate concentration that is estimated to be due to sea salt, using sodium or magnesium as tracers of sea salt.

TABLE 2.2. Data Completeness Level Criteria for Annual Summaries

Data Completeness Measure	Annual Data Completeness Level 1	2	3
%PCL			
Annual and	≥95%	≥90%	≥90%
each quarter	≥75%	≥60%	≥50%
%TP, %VSL, %VSMP			
Annual and	≥80%	≥70%	≥60%
each quarter	≥70%	≥60%	≥50%
%COLEFF			
Annual and	≥80%(70%)*	≥60%(40%)*	≥50%(30%)*
for winter and	≥80%(50%)*	≥60%(40%)*	≥50%(30%)*
spring, summer, autumn	≥80%	≥60%	≥50%
%SEASALT	≤25%	≤50%	≤75%

* The bracketed value applies to Canadian sites.

2.4 DEFINITION OF ALTERNATIVE DATA SETS USED IN STUDY

The UDDC valid sample criteria (UVSC) versus relaxed valid sample criteria (RVSC) and the UDDC data completeness rating (UDCR) versus relaxed data completeness rating (RDCR) create four subsets of sites (UVSC/UDCR, UVSC/RDCR, RVSC/UDCR and RVSC/RDCR) for both the pH and sulfate observations. The locations of the sites in the RVSC/RDCR subset are shown in Figure 2.1. The estimation technique used in this study (kriging) requires that the phenomenon be stationary in the region being investigated. For pH and wet deposition of sulfate, this stationarity requirement is not met when considering the entire United States and southern Canada as one region (Vong et. al. 1989). Therefore this study is restricted to southern Canada and eastern United States (less the southern most states). As seen in Figure 2.1, the pH observations are at the same sites as the sulfate observations with the exception of the six sites without pH observations. The number of sites in each of the subsets are shown in Table 2.3. Of the 194 sites, in the region shown in Figure 2.1, that have pH and sulfate summaries in 1986, 185 sites (95.4%) have annual pH summaries and 191 sites (98.5%) have annual sulfate summaries which meet the minimal requirements (RVSC/RDRC). When the most stringent requirements (UVSC/UDCR) are used, only 113 sites (58.2%) have annual pH summaries and 125 sites (64.4%)

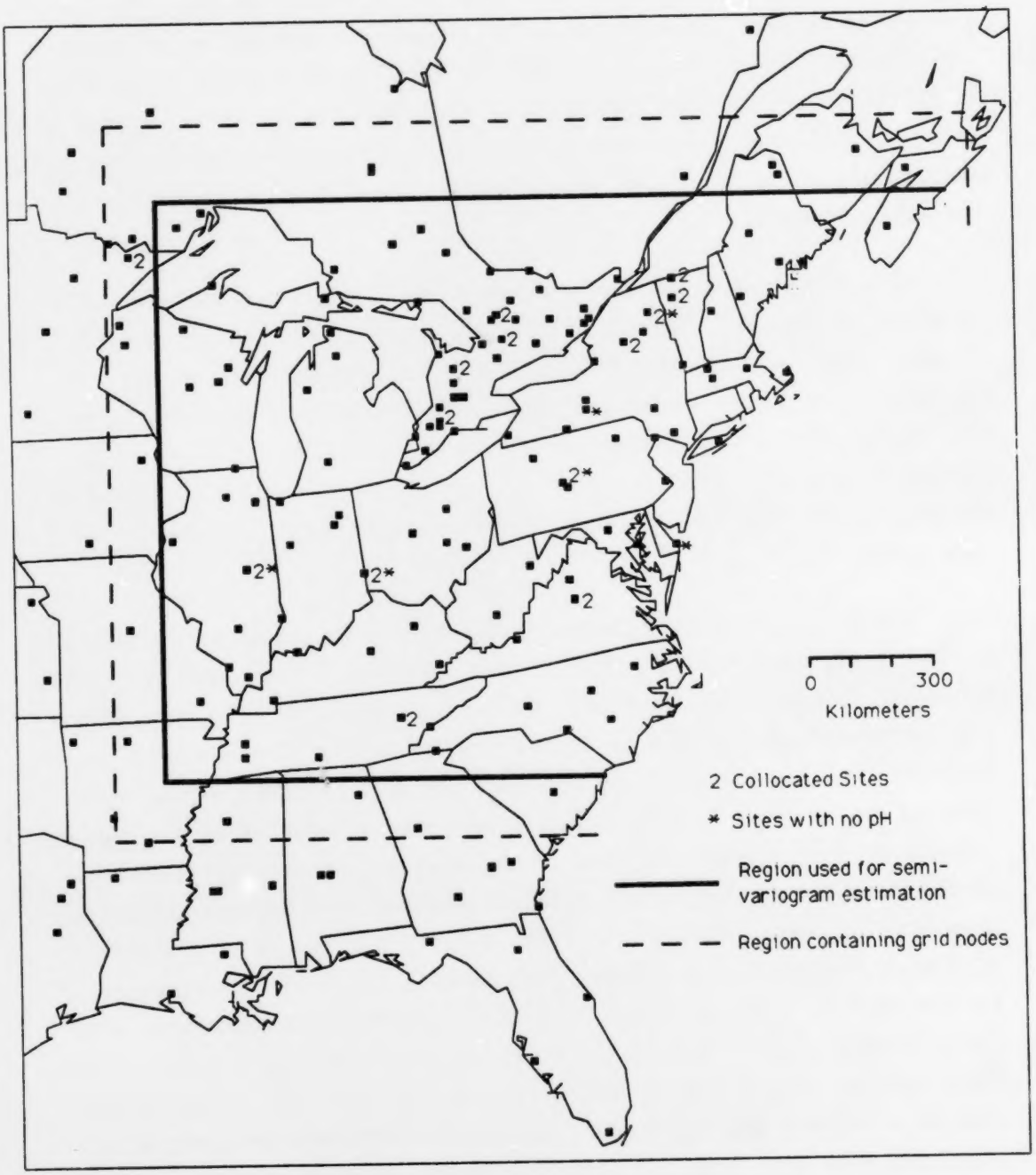

FIGURE 2.1. Location of Sites in the Relaxed Valid Sample Criteria and Relaxed Data Completeness Rating Subset

have annual sulfate summaries which meet these requirements. The difference between the UDCR and RDCR is solely in the number of sites in the subsets. The primary difference between the UVSC and RVSC subsets is that at approximately one third of the sites the summaries change in value. Additionally, the RVSC subsets have a few more sites, since more samples are included in the annual summary causing the data completeness rating to improve.

The number of sites whose observations changed and the magnitude of those changes are shown in Tables 2.4 and 2.5, for pH and sulfate respectively. As seen in Tables 2.4 and 2.5, the majority of the changes in the observations are relatively small. The 16 sites, within the region where estimates are calculated (see Figure 2.1), with the largest changes in their observations are shown in Table 2.6. As seen in this table, most of the large changes in pH and sulfate are at the same sites.

Table 2.7 shows the samples from the 16 sites shown in Table 2.6 which did not meet the UDDC valid sample criteria. There are two causes for these samples to be rejected, either the collector is open during the collection period when it is not raining (bulk) or the sample collection period violates the networks protocol by being either too long or too short. The precipitation weighted average of pH and sulfate concentration are given for most of the samples, as data validation procedures of the networks did not indicate anything unusual about the chemistry of these samples. As seen in Table 2.7, three of the sites each have samples with extremely high sulfate concentration (greater that 50 mg/l). Although there is little precipitation associated with these samples, even when precipitation weighted averages are calculated, these samples have a significant effect on the average. These unusual samples also have extremely small collection efficiencies (percent of predicted sample volume, from the rain gauge, that is contained in the actual sample). For a number of other sites, the samples that did not meet the UDDC valid sample criteria all occur contiguously in time (the NADP samples represent one week while for the APIOS-C network one sample

represents a four week period). For sites that have a seasonal trend, the loss of a month or more of data can significantly raise or lower the annual average.

A fifth subset of observations for the sulfate observations is investigated. This set consisted of the UVSC/UDCR subset with the extreme value at Parsons, West Virginia (ADS ID 075a) removed. This subset is used to demonstrate the range and magnitude of the effect that one unusual site can have.

TABLE 2.3. The Number of Sites for Each of the Four Sets of pH and Sulfate Summaries

		UVSC	RVSC
pH	RDCR	184	185
	UDCR	113	122
		UVSC	RVSC
SO_4	RDCR	190	191
	UDCR	125	133

TABLE 2.4. The Number of Sites Where pH Values Changed by the UDDC Versus Relaxed Valid Sample Criteria and the Magnitudes of Those Changes

(RVSC - UVSC)	UDCR	RDCR
(-0.127,-0.100)	1	2
(-0.100,-0.050)	3	3
(-0.050,-0.025)	1	3
(-0.025,-0.005)	11	13
(-0.005, 0.000)	10	13
no change	80	114
(0.000, 0.005)	9	14
(0.005, 0.025)	5	7
(0.025, 0.050)	2	5
(0.050, 0.096)	0	2

TABLE 2.5. The Number of Sites Where Sulfate Values Changed by the UDDC Versus Relaxed Valid Sample Criteria and the Magnitudes of Those Changes

SO_4 Concentration (mg/l)

(RVSC-UVSC)	UDCR	RDCR
(-0.27,-0.25)	0	1
(-0.25,-0.15)	0	2
(-0.15,-0.05)	2	3
(-.05,-0.00)	14	19
no change	89	120
(0.00, 0.05)	11	16
(0.05, 0.15)	9	11
(0.15, 0.25)	4	6
(0.25, 0.50)	3	4
(0.50, 0.52)	1	1

SO_4 Deposition (g/m^2)

(RVSC-UVSC)	UDCR	RDCR
(-0.33,-0.25)	0	1
(-0.25,-0.15)	0	2
(-0.15,-0.05)	2	2
(-0.05,-0.00)	14	20
no change	89	120
(0.00, 0.05)	11	16
(0.05, 0.15)	8	10
(0.15, 0.25)	3	4
(0.25, 0.50)	5	7
(0.50, 0.53)	1	1

TABLE 2.6. The Sixteen Sites with the Largest Changes in Their pH and/or Sulfate Concentrations as a Result of Using the Relaxed Versus UDDC Valid Sample Criteria

ADS Site ID	Network	Sitename	Precip (cm)	DCR UV	DCR RV	% Total Precip UV	% Total Precip RV	Number of Samples UV	Number of Samples RV	pH UV	pH RV	pH Difference
032a	NADP	Kellogg, Michigan	125	RD	RD	60	89	29	36	4.372	4.400	+0.028
043b	NADP	Whiteface, New York	117	RD	UD	77	84	40	44	4.373	4.369	0.004
047a	NADP	Jasper, New York	83	RD	UD	75	81	41	42	4.261	4.205	-0.056
073a	NADP	Horton Station, Virginia	96	RD	RD	63	75	32	34	4.383	4.418	+0.035
077a	NADP	Spooner, Wisconsin	79	UD	UD	92	94	36	38	4.898	4.878	-0.020
163a	NADP	Caribou, Maine	88	UD	UD	99	100	48	50	4.617	4.604	-0.013
168a	NADP	Huntington, New York	109	RD	UD	75	83	39	46	4.351	4.325	-0.026
187a	APIOS-C	Uxbridge, Ontario	94	RD	RD	65	73	8	10	4.251	4.282	+0.031
188a	APIOS-C	Wilberforce, Ontario	99	RD	UD	75	94	10	12	4.299	4.342	+0.043
192a	APIOS-C	Smith's Falls, Ontario	97	RD	RD	86	100	11	12	4.323	4.289	-0.034
208a	APIOS-C	Lac Le Croix, Ontario	58	RD	RD	68	89	7	9	5.016	4.889	-0.127
241a	UAPSP	Gaylord, Michigan	85	UD	UD	89	97	73	75	4.511	4.454	-0.057
250a	NADP	Big Meadows, Virginia	105	RD	RD	62	69	23	27	4.438	4.410	-0.028
276a	NADP	Cadwell, Massachuetts	113	RD	UD	82	96	33	37	4.307	4.310	+0.003
420a	NADP	Vincennes, Indiana	115	RD	UD	83	94	31	38	4.386	4.289	-0.097
495a	APIOS-C	Moosonee, Ontario	62	RD	RD	75	94	6	9	4.852	4.947	+0.095

Legend:

Precip	Total annual precipitation
DCR	Data completeness rating
UD	Meets UDDC data completeness rating
RD	Meets relaxed data completeness rating
UV	Using the UDDC valid sample criteria
RV	Using the relaxed valid sample criteria
% Total Precip	Percentage of the total annual precipitation represented by the valid samples
Samples	Number of valid samples

TABLE 2.6 (Continued).

ADS Site ID	DCR UV	DCR RV	% Total Precip UV	% Total Precip RV	Number of Samples UV	Number of Samples RV	SULFATE Concentration (mg/l) UV	Concentration (mg/l) RV	Concentration (mg/l) Difference	DEPOSITION (g/m^2) UV	DEPOSITION (g/m^2) RV	DEPOSITION (g/m^2) DIFFERENCE
032a	RD	RD	60	89	29	36	2.743	2.475	-0.268	3.416	3.082	-0.334
043b	RD	RD	77	84	40	44	1.967	2.184	+0.217	2.308	2.561	+0.253
047a	RD	UD	75	81	41	42	2.564	3.021	+0.458	2.139	2.521	+0.382
073a	RD	RD	63	75	32	34	2.463	2.238	-0.225	2.370	2.154	-0.216
077a	UD	UD	92	94	36	38	1.436	1.758	+0.322	1.134	1.388	+0.254
163a	UD	UD	99	100	48	50	1.319	1.836	+0.517	1.156	1.609	+0.453
168a	RD	UD	75	83	39	45	2.079	2.190	+0.111	2.261	2.382	+0.121
187a	RD	RD	65	73	8	10	3.573	3.341	-0.232	3.348	3.131	-0.217
188a	UD	UD	65	84	10	12	2.816	2.818	+0.002	2.794	2.796	+0.002
192a	RD	RD	62	69	23	27	2.955	3.114	+0.159	2.864	3.018	+0.154
208a	RD	RD	78	100	9	11	1.349	1.383	+0.034	0.789	0.809	+0.020
241a	UD	UD	89	97	73	75	1.586	1.824	+0.238	1.340	1.541	+0.201
250a	RD	RD	62	69	23	27	1.925	2.184	+0.259	2.013	2.284	+0.271
276a	RD	UD	87	96	42	44	2.078	2.215	+0.137	2.352	2.508	+0.156
420a	RD	UD	83	94	31	38	2.620	3.081	+0.461	3.020	3.551	+0.531
495a	RD	RD	67	83	6	8	1.442	1.406	-0.036	0.887	0.865	-0.022

Legend:

Precip	Total annual precipitation
DCR	Data completeness rating
UD	Meets UDDC data completeness rating
RD	Meets relaxed data completeness rating
UV	Using the UDDC valid sample criteria
RV	Using the relaxed valid sample criteria
% Total precip	Percentage of the total annual precipitation represented by the valid samples
Ssmples	Number of valid samples

TABLE 2.7. The Samples Within the 16 Sites (Shown in Table 2.6) Which Did Not Meet the UDDC Valid Sample Criteria

ADS SITE ID	N	CAUSE	PRECIP	% TOTAL PRECIP	pH	SULFATE CONC (mg/l)	COMMENTS
032a	1	period	25.6	20.6	4.600	1.450	no sample volume
	6	period	11.2	9.0	4.334	3.040	
0.43b	1	bulk	3.5	3.0	4.190	7.790	July
	3	bulk	4.3	3.6	4.506	2.152	July
047a	1	bulk	4.4	5.3	3.770	9.560	
073a	2	period	12.0	12.4	4.662	1.102	
077a	1	bulk	0.8	1.0	6.44	1.250	
	1	bulk	0.3	0.4	3.75	74.050	5.8% collection efficiency
163a	2	bulk	0.9	1.0	4.726	51.995	11.2% and 24.8% collection efficiency
168a	4	bulk	5.5	5.2	4.158	2.441	February and March
	2	bulk	3.0	2.8	4.182	4.734	
	1	bulk	0.1	0.1	3.860		
187a	2	period	7.5	8.0	4.666	1.478	
188a	2	bulk	18.7	18.9	4.751	2.826	
192a	1	bulk	13.5	13.9	4.120	4.100	
208a	1	period	2.7	4.7	5.020	0.800	
	1	period	9.9	16.9	4.570	1.700	35.1% collection efficiency
241a	2	period	6.1	7.3	4.053	4.744	
250a	2	bulk	5.8	5.6	4.542	1.540	March and April
	2	bulk	2.2	2.1	4.044	11.321	March and April
276a	1	bulk	2.5	2.2	6.96	5.824	
	1	bulk	8.2	7.2	4.23	2.750	
420a	6	bulk	12.4	10.8	4.556	3.906	February and March
	1	bulk	0.5	0.4	2.680	69.320	2.9% collection efficiency
495a	1	period	2.2	3.6	4.640		
	1	period	2.2	3.5	7.120	1.100	November
	1	period	7.8	12.7	6.210	1.300	December, 2.0% collection efficienc

3.0 KRIGING

To investigate the effects of using the four different subsets of the observations, the observations are interpolated unto a regular grid using a variation of kriging. Kriging has often been the tool used to make predictions of a spatial phenomenon (e.g. sulfate deposition) at unobserved sites (e.g. a grid node). Kriging's popularity is based on the fact that the estimates it produces are 'sensible' and it also produces a variance that is often used in setting confidence intervals about the estimates.

3.1 KRIGING ASSUMPTIONS

Let $Z(\underline{x})$ be a realization of a spatial phenomenon. For example, $Z(\underline{x})$ can be the sulfate deposition at a site and $\underline{x}$ is the location of the site in two dimensional space ($\underline{x} = (x,y)$). 'Simple' Kriging assumes that the increments (difference between the sulfate deposition at two sites), $[Z(\underline{x}') - Z(\underline{x})]$, are stationary in the weak sense. That is,

$$E[Z(\underline{x}') - Z(\underline{x})] = 0 \qquad (1)$$

and

$$VAR[Z(\underline{x}') - Z(\underline{x})] = 2\gamma(h) \qquad (2)$$

where

h = distance between $\underline{x}$ and $\underline{x}'$

$\gamma(h)$ = semi-variogram .

Equation (1) states that the expected difference between the two sites is zero or that the expected sulfate depositions are constant over the region of interest. Equation (2) states that the increment has a variance and this variance is a function (called the semi-variogram) only of the distance between the two sites.

When there is a systematic change (drift or trend) in the spatial phenomenon, then

$$E[Z(\underline{x})] = m(\underline{x}) \tag{3}$$

where $m(\underline{x})$ is usually modeled as a low order polynomial. Now, using equation (3),

$$E[Z(\underline{x}') - Z(\underline{x})] = m(\underline{x}') - m(\underline{x}) . \tag{4}$$

and

$$VAR[Z(\underline{x}') - Z(\underline{x})] = 2\gamma(h) - [m(\underline{x}') - m(\underline{x})]^2 . \tag{5}$$

Thus, the increments no longer have a constant expected value and the variance of the increments is a function of both the semi-variogram and the drift. Now the variance of the increments cannot be modeled by the semi-variogram alone. The problem at this point is that to be able to estimate the drift, the semi-variogram needs to be known, and to be able to estimate the semi-variogram, the drift needs to be known. Unfortunately, neither are known.

In practice, often the drift is ignored. There are two common justifications given for ignoring the drift. First, the actual estimates derived from kriging only uses a subset of the sites near the point being estimated, thus if the drift is 'small' in the 'neighborhood' of the point being estimated then the drift's effect on the estimates will be negligible. The second justification is that 'what's drift to one person is correlation to the next.'

3.2 SEMI-VARIOGRAM ESTIMATION

As seen in equation (2), under the assumption that the increments are stationary in the weak sense, the variance of the increments are modeled by the semi-variogram. The semi-variogram model must be of a form so that the variance is non-negative.

Five of the more common semi-variogram models which give non-negative values are:

1. Power Model

$$\gamma(h) = b|h|^p \qquad \text{for } 0 < p < 2$$

(when p=1, the semi-variogram is simply a linear model)

2. Spherical Model

$$\gamma(h) = C\left[\frac{3}{2}\frac{|h|}{r} - \frac{1}{2}\frac{|h|^3}{r^3}\right] \qquad \text{for } |h| \le r$$

$$\gamma(h) = C \qquad \text{for } |h| > r$$

3. Cubic Model

$$\gamma(h) = C\left[7\frac{|h|^2}{r^2} - \frac{35}{4}\frac{|h|^3}{r^3} + \frac{7}{2}\frac{|h|^5}{r^5} - \frac{3}{4}\frac{|h|^7}{r^7}\right] \qquad \text{for } |h| \le r$$

$$\gamma(h) = C \qquad \text{for } |h| > r$$

4. Exponential Model

$$\gamma(h) = C\left[1 - e^{-|h|/(r/3)}\right]$$

5. Gaussian Model

$$\gamma(h) = C\left[(1 - e^{-|h|^2/(r/2)^2}\right]$$

In the above equations, r equals the range of the semi-variogram and C equals the sill. The range can be thought of as the 'zone of influence'. If the distance between two sites is less than the range, then the value of one site influences the value of the other site. If the distance between two sites is greater than the range, then the sites are independent. The sill is the bound on the semi-variogram and provides an estimate of the overall variability. The power model does not have a range or a sill. The exponential and gaussian models never reach their sill. Figure 3.1 gives a comparison of these semi-variogram models where the sill and range are one for all the models except the

power models where b is set to one and the semi-variogram is truncated at one at distance one. As seen in Figure 3.1, a wide range of semi-variograms can be modeled using these five models.

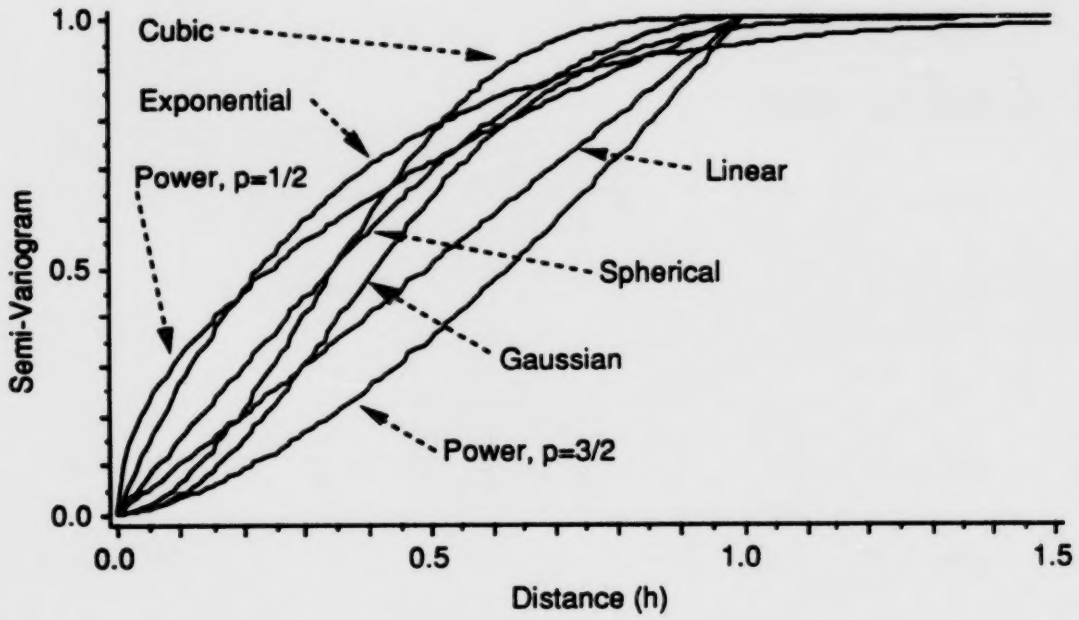

FIGURE 3.1. Semi-Variogram Models Where the Sill and Range are One For All the Models Except the Power Models Where "b" is Set to One and the Semi-Variogram is Truncated at One at Distance of One

When h is zero, g(0) must also be equal to zero. However, if the semi-variogram does not tend to zero for measurements taken at arbitrarily close points, then there is a discontinuity of the semi-variogram at the origin. This discontinuity is called the nugget effect. If there is a nugget effect, the variogram model is adjusted to take it into account. For example, if the model is linear with a nugget of size C_0 (the intercept) then

$$\gamma(h) = b|h| + C_0 \qquad \text{for } |h| > 0$$

$$\gamma(h) = 0 \qquad \text{for } |h| = 0 \ .$$

The semi-variogram is estimated by

$$\hat{\gamma}(h) = \frac{1}{2N(h)} \sum_{i=1}^{N(h)} [Z(\underline{x}_i + h) - Z(\underline{x}_i)]^2 \qquad (6)$$

where

$Z(\underline{x}_i + h) - Z(\underline{x}_i)$ = difference between a pair of observations which are a distance h apart

$N(h)$ = number of pairs of points actually taken into the sum.

In practice h is a range of distances.

3.3 KRIGING ESTIMATOR

The Kriging estimator is

$$\hat{Y}_0 = \sum_{i=1}^{n} \lambda_i Z(\underline{x}_i) \qquad (7)$$

where

$\hat{Y}_0$ = the Kriging estimator at grid node $\underline{x}_0$

λ_i = kriging weights

$Z(\underline{x}_i)$ = the observed sulfate deposition at site $\underline{x}_i$

n = the number of sites used in the estimator.

The number of sites used in the estimator, n, is only a small fraction of the total number of sites (generally between 8 and 16). Only 'close' observations are used to reduce the size of the matrices that need to be manipulated. As long as the semi-variogram model has a small nugget as compared to the sill, then the weights decrease rapidly with distance from $\underline{x}_0$ and thus observations that are 'far' from $\underline{x}_0$ have negligible weight.

The 'simple' Kriging variance is

$$\sigma_k^2 = 2\sum_{i=1}^{n} \lambda_i \gamma(\underline{x}_i,\underline{x}_0) - \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j \gamma(\underline{x}_i,\underline{x}_j)$$

where

$\gamma(\underline{x}_i,\underline{x}_j)$ = semi-variogram, g(h) where h is the distance between $\underline{x}_i$ and $\underline{x}_j$.

If the semi-variogram has a sill and there is no drift, the Kriging variance may be stated in terms of variances and covariances.

$$\sigma_k^2 = = \sum_{i=1}^{n}\sum_{j=1}^{n} \lambda_i\lambda_j \sigma(\underline{x}_i,\underline{x}_j) - 2\sum_{i=1}^{n} \lambda_i \sigma(\underline{x}_i,\underline{x}_0) + \sigma^2$$

where

$\sigma(\underline{x}_i,\underline{x}_j)$ = covariance between $\underline{x}_i$ and $\underline{x}_j$

$= \sigma^2 - \gamma(\underline{x}_i,\underline{x}_j)$

σ^2 = variance of Y_0 (sill). (7)

3.4 GENERALIZED LEAST SQUARES (GLS) REGRESSION

Least squares regression assumes that the errors in the observations are independent. That is, the deviations from a trend surface fit using least squares regression and the actual observations are independent. If it assumed that these errors are not independent, then generalized least squares regression can be used to estimate the trend surface. For example, in kriging the dependence in the errors is assumed to be a function only of the distance between the observations. Because these errors are related, they also form a 'surface' that fits on top of the trend surface. Therefore, it makes sense to also estimate the error 'surface' and then add it to the trend surface.

3.5 DERIVATION OF THE GLS ESTIMATOR

The GLS model is

$$\underline{Y} = \mathbf{X}\underline{\beta} + \underline{\varepsilon}$$

where

$$\underline{Y}' = (Y_1, Y_2, \ldots, Y_n)$$

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & y_1 & \cdot & \cdot & \cdot & f^m(\underline{x}_1) \\ 1 & x_2 & y_2 & \cdot & \cdot & \cdot & f^m(\underline{x}_2) \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & x_n & y_n & \cdot & \cdot & \cdot & f^m(\underline{x}_n) \end{bmatrix}$$

$f^m(\underline{x}_i)$ = a low-order polynomial of $\underline{x}_i$

$$\underline{\beta}' = (\beta_1, \beta_2, \ldots, \beta_m)$$

$\underline{\varepsilon} \sim (\underline{0}, \sigma^2\mathbf{V})$ (i.e. distributed with mean zero and covariance matrix $\sigma^2\mathbf{V}$, the form of the distribution (e.g. Gaussian) need not be specified until required for computing confidence intervals, etc.)

$$\mathbf{V} = \begin{bmatrix} \sigma(\underline{x}_1,\underline{x}_1) & \sigma(\underline{x}_1,\underline{x}_2) & \cdot & \cdot & \cdot & \sigma(\underline{x}_1,\underline{x}_n) \\ \sigma(\underline{x}_2,\underline{x}_1) & \sigma(\underline{x}_2,\underline{x}_2) & \cdot & \cdot & \cdot & \sigma(\underline{x}_2,\underline{x}_n) \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \sigma(\underline{x}_n,\underline{x}_1) & \sigma(\underline{x}_n,\underline{x}_2) & \cdot & \cdot & \cdot & \sigma(\underline{x}_n,\underline{x}_n) \end{bmatrix}$$

σ^2 is the sill of the semi-variogram.

Then

$$\hat{\underline{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\underline{Y}$$

$$\hat{\sigma}^2 = \frac{1}{n-m}(\underline{Y} - \mathbf{X}\hat{\underline{\beta}})'\mathbf{V}^{-1}(\underline{Y} - \mathbf{X}\hat{\underline{\beta}})$$

$$\text{VAR}[\hat{\underline{\beta}}] = \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1} .$$

Now, the value of the realization at the unobserved location $\underline{x}_0$ is

$$Y_0 = \underline{X}_0'\underline{\beta} + \varepsilon_0$$

where

$$\underline{X}_0' = [\ 1, x_0, y_0, \ldots, f^m(\underline{x}_0)]$$

$$\varepsilon_0 \sim (0, \sigma^2)$$

$$\text{COV}[\underline{\varepsilon}, \varepsilon_0] = \sigma^2\underline{V}_0$$

$$\underline{V}_0' = [\ \sigma(\underline{x}_1, \underline{x}_0), \sigma(\underline{x}_2, \underline{x}_0), \ldots, \sigma(\underline{x}_n, \underline{x}_0)] .$$

Then,

$$\begin{bmatrix} \varepsilon_0 \\ \underline{\varepsilon} \end{bmatrix} \sim \left(\begin{bmatrix} 0 \\ \underline{0} \end{bmatrix}, \sigma^2 \begin{bmatrix} 1 & \underline{V}_0' \\ \underline{V}_0 & \mathbf{V} \end{bmatrix} \right)$$

so

$$\varepsilon_0 | \underline{\varepsilon} \sim (\underline{V}_0'\mathbf{V}^{-1}\underline{\varepsilon},\ \sigma^2(1 - \underline{V}_0'\mathbf{V}^{-1}\underline{V}_0)) .$$

Thus,

$$\hat{Y}_0 = \underline{X}_0'\hat{\underline{\beta}} + \hat{\varepsilon}_0$$

where

$$\hat{\varepsilon}_0 = \underline{V}_0'\mathbf{V}^{-1}\hat{\underline{\varepsilon}} .$$

Then,

$$\hat{Y}_0 = \underline{X}_0'\hat{\underline{\beta}} + \underline{V}_0'\mathbf{V}^{-1}\hat{\underline{\varepsilon}}$$

$$= \underline{X}_0'\hat{\underline{\beta}} + \underline{V}_0'\mathbf{V}^{-1}(\underline{Y} - \mathbf{X}\hat{\underline{\beta}})$$

$$= \underline{V}_0'\mathbf{V}^{-1}\underline{Y} + \underline{X}_0'\hat{\underline{\beta}} - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X}\hat{\underline{\beta}}$$

$$= \underline{V}_0'\mathbf{V}^{-1}\underline{Y} + (\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})\hat{\underline{\beta}}$$

$$= \underline{V}_0'\mathbf{V}^{-1}\underline{Y} + (\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\underline{Y}$$

$$= [\underline{V}_0'\mathbf{V}^{-1} + (\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}]\underline{Y}$$

$$= \underline{\lambda}'\underline{Y}$$

where $\underline{\lambda}$ is the vector of kriging weights.

Now,

$$VAR[\hat{Y}_0] = VAR[\underline{\lambda}'\underline{Y}] = \underline{\lambda}'VAR[\underline{Y}]\underline{\lambda} = \sigma^2\underline{\lambda}'\mathbf{V}\underline{\lambda}$$

$$= \sigma^2\underline{V}_0'\mathbf{V}^{-1}\underline{V}_0 + \sigma^2(\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}(\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})'$$

$$+ 2\sigma^2\underline{V}_0'\mathbf{V}^{-1}\mathbf{X}(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}(\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})',$$

$$VAR[Y_0] = \sigma^2$$

and

$$COV[\hat{Y}_0, Y_0] = COV[\underline{\lambda}'\underline{Y}, Y_0] = \underline{\lambda}'COV[\underline{Y}, Y_0] = \sigma^2\underline{\lambda}'\underline{V}_0$$

$$= \sigma^2[\underline{V}_0'\mathbf{V}^{-1} + (\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}]\underline{V}_0$$

$$= \sigma^2\underline{V}_0'\mathbf{V}^{-1}\underline{V}_0 + \sigma^2(\underline{X}_0' - \underline{V}_0'\mathbf{V}^{-1}\mathbf{X})(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\underline{V}_0$$

So,

$$VAR[\hat{Y}_0 - Y_0] = VAR[\hat{Y}_0] + VAR[Y_0] - 2COV[\hat{Y}_0, Y_0]$$

thus,

$$\mathrm{VAR}[\,\hat{Y}_0 - Y_0\,] = \sigma^2 - \sigma^2 \underline{V}_0' \mathbf{V}^{-1} \underline{V}_0$$

$$+ \sigma^2 (\underline{X}_0' - \underline{V}_0' \mathbf{V}^{-1} \mathbf{X})(\mathbf{X}' \mathbf{V}^{-1} \mathbf{X})^{-1} (\underline{X}_0' - \underline{V}_0' \mathbf{V}^{-1} \mathbf{X})' \,.$$

This is the kriging variance.

3.6 WITHIN-SITE VARIATION

The nugget effect in kriging is often attributed to the within-site variation. The practical result of using the nugget effect in kriging is to force the surface through the observations. That is, the kriging estimate at a site which has an observation is that observation. Thus the surface has 'spikes' wherever there are observations. These 'spikes' have no surface area associated with them, they are a jump discontinuity at the site of the observation. Additionally, the sites with duplicate observations must be preprocessed (usually the mean observation is calculated), since only one observation per site can be used.

In the GLS estimation procedure, the within-site variation is accounted for by an additional parameter in the model,

$$\underline{Y} = \mathbf{X}\beta + \underline{\varepsilon} + \underline{\eta}$$

where

$$\underline{\eta} \sim (0, \sigma_w^2 \mathbf{I})$$

$\underline{\eta}$ and $\underline{\varepsilon}$ are uncorrelated.

These two sources of error can be combined so that

$$\underline{Y} = \mathbf{X}\beta + \underline{\nu}$$

where

$$\underline{\nu} \sim (0, \sigma^2 \mathbf{V} + \sigma_w^2 \mathbf{I}) \,.$$

Then in the derivations shown in Section 3.5, $\sigma^2\mathbf{V}$ is replaced by $\sigma^2\mathbf{V} + \sigma_w^2\mathbf{I}$. Note that $\underline{V}_0$ is not changed.

This formulation assumes that the within-site variation is the same for all sites. However, if the information is available, each site could have it's own within-site variation and $\sigma_w^2\mathbf{I}$ is simply replaced with a diagonal matrix, with the diagonal elements being the within-site variation at each site.

By using this within-site variation formulation, the only time the estimate will differ from the kriging estimate using the nugget is at the observation. Now the estimate is no longer the same as the observation. Additionally, sites with duplicate observations do not need to be preprocessed. The algorithm in essence uses their mean.

If there is no within-site variation, then the estimate at a site where there is an observation will be that observation. That is, the model assumes that there is no variation (or error) in the data. In the original application of kriging to ore reverse estimation, this assumption may be valid. However, in applying kriging to wet deposition summaries, the assumption that the data at a site has no inherent variability or error does not appear to be valid.

3.7 ADVANTAGES OF GLS APPROACH

When the variance-covariance matrix is specified using a function that is dependent on distance, the GLS approach is kriging. However, the GLS approach has the flexibility to both investigate the phenomenon of interest and to add additional information to the model.

Often one semi-variogram does not fit the entire region of interest. Currently, to get around this problem, the region is divided into several smaller regions. The boundaries of the sub-regions are usually artificial and ad-hoc procedures must be used to blend the results for the separate sub-regions together. By doing a 'moving' GLS, where only a relatively small number of observations near the point of interest are used in the estimation process, the changes in the 'sill'

of the semi-variogram can be investigated over the region of interest. Additionally, by using a 'moving' approach, the problem with the boundaries of the arbitrarily chosen regions no longer exist.

The GLS approach allows other information to be added to the model. For example, there are some pollutants that are highly correlated with population density (e.g. automobile exhausts). Additionally, information about population density across the United States can be obtained or well estimated with census information. By adding this population information to the model, observations in urban areas will not cause overestimation in nearby rural areas and observations in rural areas will not cause underestimation in nearby urban areas.

4.0 VARIOGRAM ESTIMATES

From previous studies it is known that one semi-variogram does not fit the entire region shown in Figure 2.1. The shape of the semi-variograms for pH and sulfate precipitation concentration and deposition are primarily due to the 'depression', for pH, and 'hump', for sulfate, in the surface that is centered around northeastern West Virginia. These surfaces maintain about the same slopes within the smaller region shown in Figure 2.1. Outside this region the slopes change markedly (increases with pH and decreases with sulfate) and thus the semi-variogram model also changes.

Because our concern in this paper is about the effects of changing criteria for data, we will only look at the region where one variogram reasonably works. Because the exact boundary for this region is not known, the semi-variograms are calculated using only the sites within the smallest region. However, the grid is expanded to the larger region and any site shown in Figure 2.1 is potentially used in the estimate.

Figure 4.1 shows the raw semi-variograms and the estimated models for pH, sulfate concentration and sulfate deposition. As seen in this figure the semi-variograms do not change very much between the four different subsets. Therefore, one semi-variogram model can be used for all four subsets. The 'nugget' that is observed at the origin of these semi-variograms is used as the estimates of the within-site variation. Additionally, since we use the GLS method the semi-variogram model is converted to it's covariance equivalent (see equation 7). The pH has a linear model with a sill of 0.03 (pH units)^2, a range of 1280 kilometers and a within-site variance of 0.002 (pH units)^2. The range of the linear model is artificially set beyond the actual range used since the covariance model needs a range. The sulfate concentration has an exponential model with a sill of 0.44, (mg/l)^2 a range of 1150 kilometers and a within-site variance of 0.02 (mg/l)^2. The sulfate deposition has an exponential model with a sill of 0.70 (g/m^2)^2, a range of 960 kilometers and a within-site variance of 0.03 (g/m^2)^2. The

exponential model actually never reaches the sill, the range given above is the distance where the model is 95 percent of the sill.

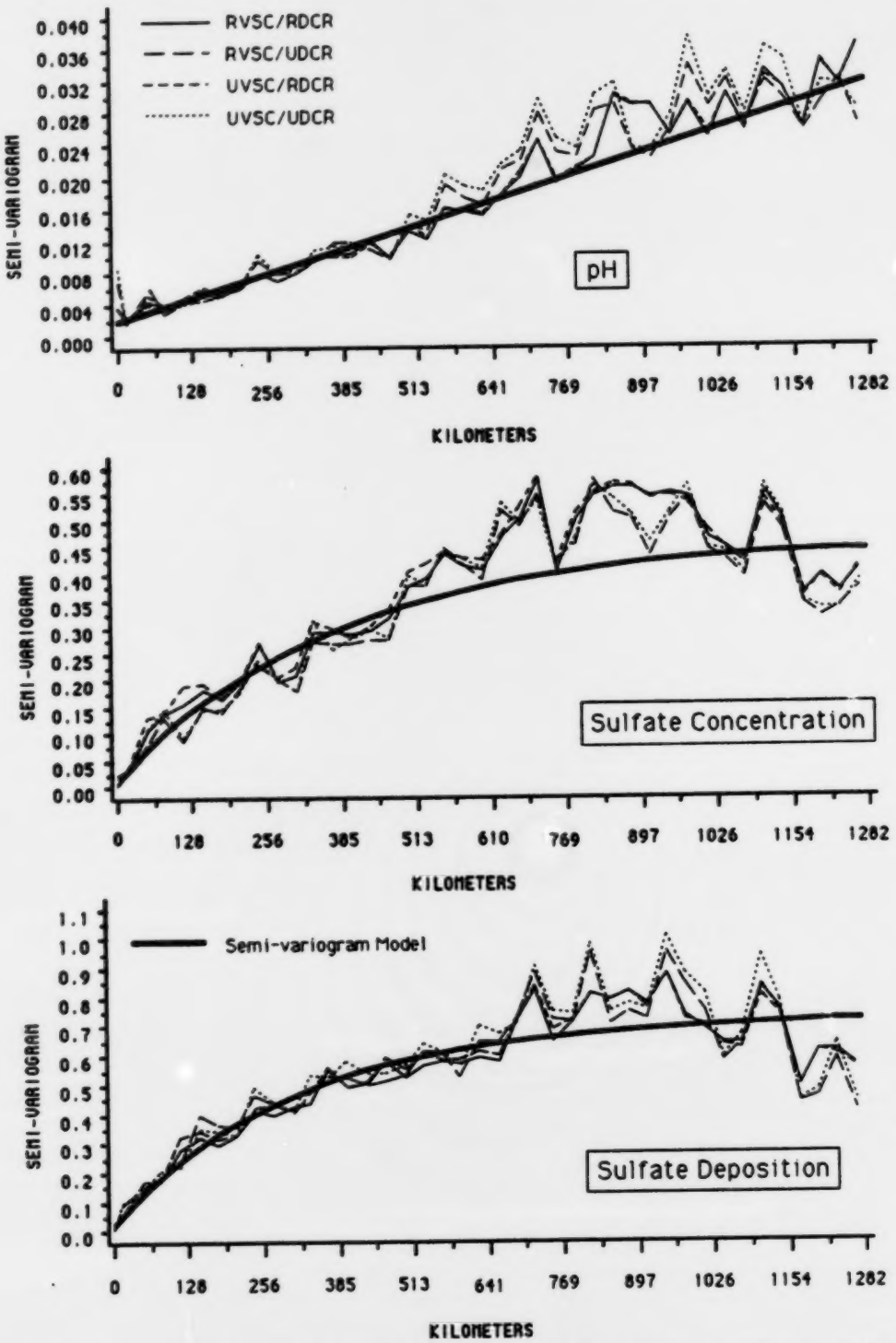

FIGURE 4.1. Semi-variogram for each of the Subsets of pH, Sulfate Concentration and Sulfate Distributions

5.0 RESULTS

The GLS variation of kriging, described in section 3, is used to estimate the pH, sulfate concentration, and sulfate deposition for each of the subsets at grid nodes of a regular square grid. This procedure uses the eight closest sites to the grid node in the estimate. The grid nodes are 32 kilometers apart and the area of the grid, shown in Figure 2.1, consists of 3669 nodes. This grid is then contoured using bilinear interpolation in SAS (procedure gcontour).

The contour maps of the pH and sulfate concentration and deposition show, in broad terms, the effects of using different subsets of the observations. Additionally, contour maps of the differences between several of the different subsets at each grid node are prepared. These maps show the 'local' effects, both extent and magnitude, of using different subsets of observations.

5.1 CONTOUR MAPS OF THE ESTIMATES

Figures 5.1, 5.2, and 5.3 show the contoured estimates of pH, sulfate concentration and deposition, respectively, using the UVSC/UDCR subsets of observations. These maps are shown for two reasons. First, they are the maps that use the observations that meet the current, and most stringent, sample validity and data completeness criteria. Thus, the effects of using different subsets of observations are judged relative to these maps. Secondly, these maps are large enough to include details, such as the contour levels, that become lost as the maps are reduced in size for comparisons. As seen in Figures 5.1 and 5.2, the pH and sulfate concentrations have relatively smooth contour maps. However, as seen in Figure 5.3, sulfate deposition's contour map has several mounds and depressions. The sulfate deposition is the multiple of the sulfate concentration and total precipitation. The mounds and depressions in the sulfate deposition contour map are due to precipitation gradients that are not parallel to the concentration gradients or to local precipitation that is unusually high or low compared to neighboring sites.

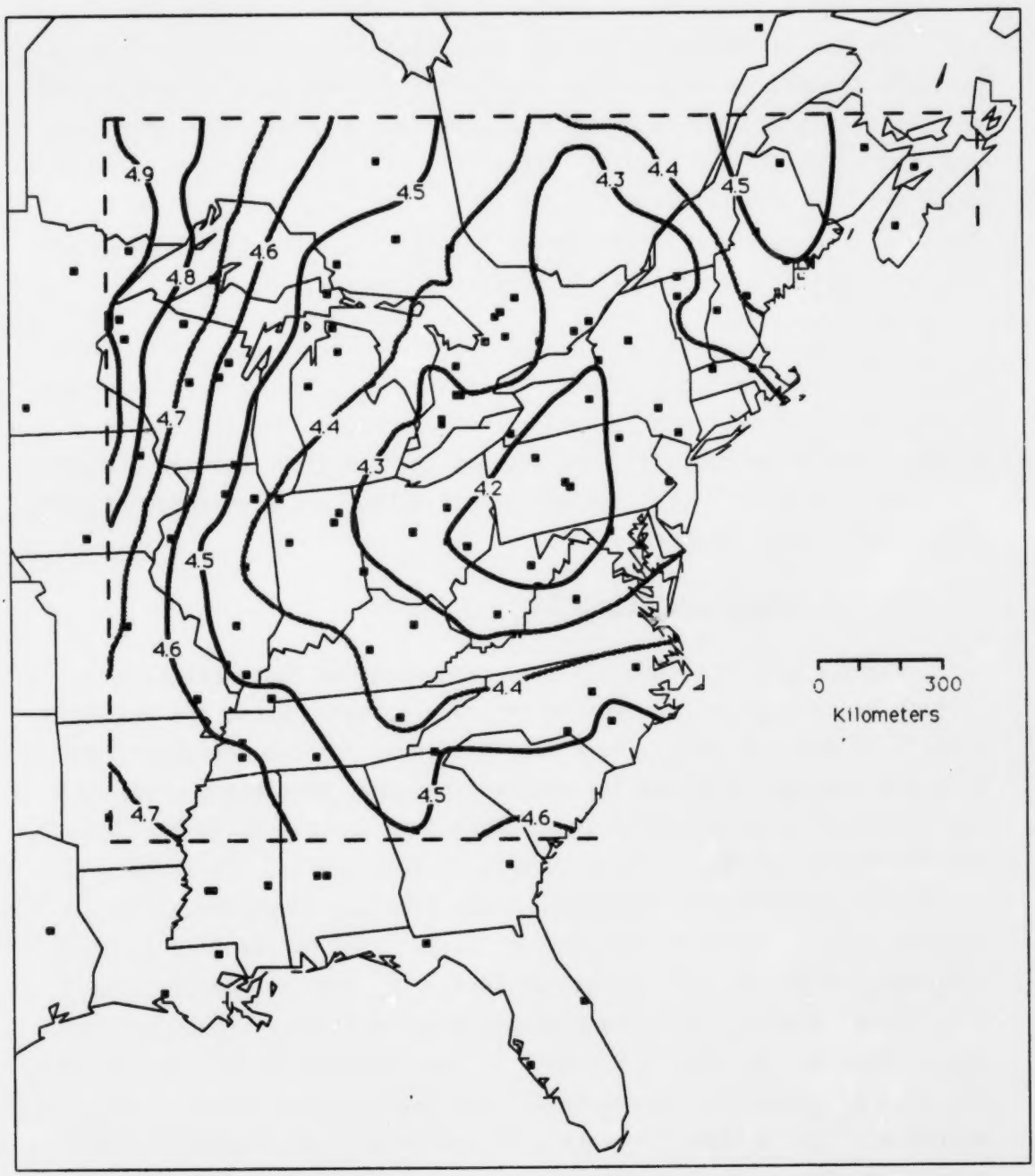

FIGURE 5.1. Contours of pH Estimates Using the UDDC Valid Sample Criteria/ UDDC Data Completeness Rating Subset

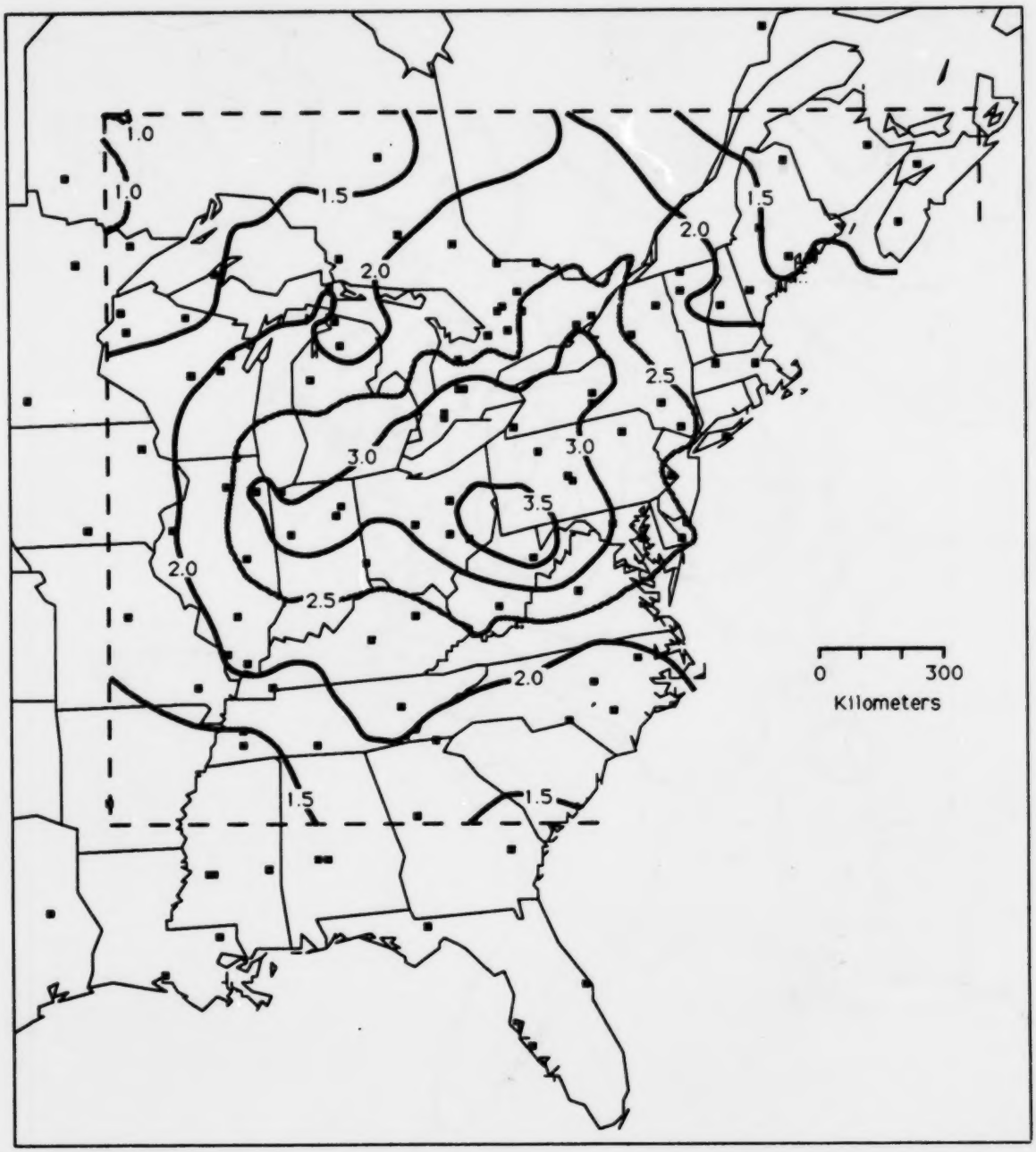

FIGURE 5.2. Contours of Sulfate Concentrations (mg/l) Estimates Using the UDDC Valid Sample Criteria/UDDC Data Completeness Rating Subset.

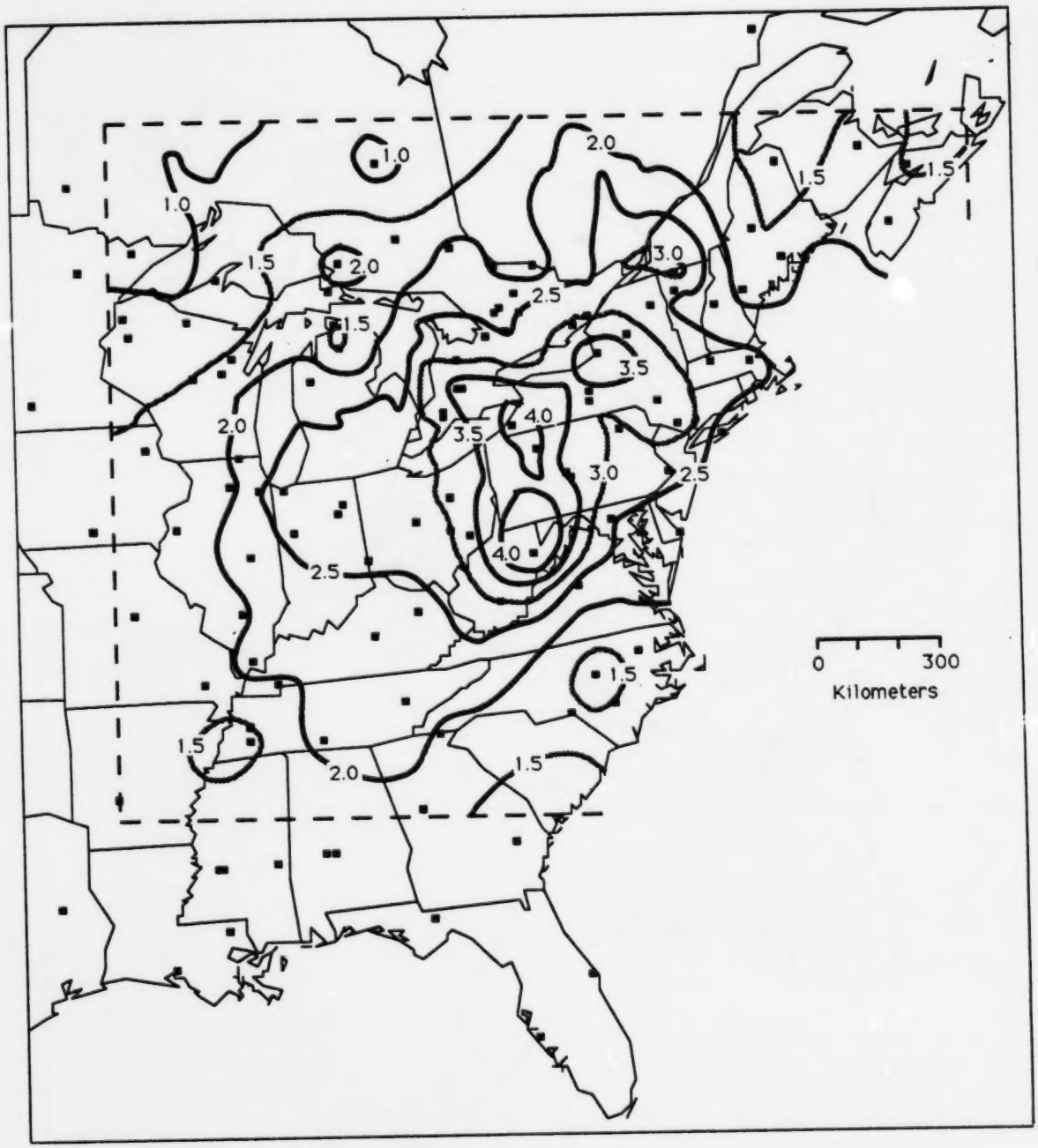

FIGURE 5.3. Contours of Sulfate Depositions (g/sq m) Estimates Using the UDDC Valid Sample Criteria/UDDC Data Completeness Rating Subset

Figures 5.4, 5.5, and 5.6 show the contoured estimates of pH, sulfate concentration and deposition, respectively, using all four subsets of observations. In these figures, the number of sites used increases from left to right (UDCR versus RDCR) and the value of the observations change from top to bottom (UVSC versus RVSC).

The pH estimates (see Figure 5.4) increase in Ontario and Quebec when the number of sites used increase, from UDCR to RDCR. This region has few sites, so the addition of a few more sites has a profound effect on the contours. The additional sites also produced increases in pH in northeastern New York, northern Virginia, southern West Virginia, eastern Tennessee, northern Alabama, northern Mississippi and Arkansas decreases in North Carolina, eastern Wisconsin, and southwestern Indiana. Along the border of Pennsylvania and New York the value of the observation at one site (ADS ID 047a; NADP; Jasper, New York) has a profound effect when the UVSC is used versus the RVSC. This site is not in the UVSC/UDCR subset.

The sulfate concentration estimates (see Figure 5.5) change in Ontario and Quebec when the number of sites used increase, from UDCR to RDCR. As with pH this region has few sites, so the addition of a few more sites has a profound effect on the contours. However, for sulfate concentration there is a decrease to the north and an increase in the south. The increase in sites have a profound effect on the largest contour, 3.5 mg/l. When the UDCR is used, this contour is confined to northern West Virginia, southeastern Ohio and southwestern Pennsylvania. However with the additional sites in southern Ontario, when the RDCR is used, this contour now stretches approximately three hundred of kilometers north-northwest into southern Ontario. There are also increases in southern Indiana and western North Carolina and a decrease in northern Virginia. The change in the values of the observations, UVSC versus RVSC, has the effect of increasing the estimates on the southern border between Indiana and Illinois and in Maine. Again site 047a, along the Pennsylvania and New York border also has a noticeable effect in the UVSC/RDCR subset.

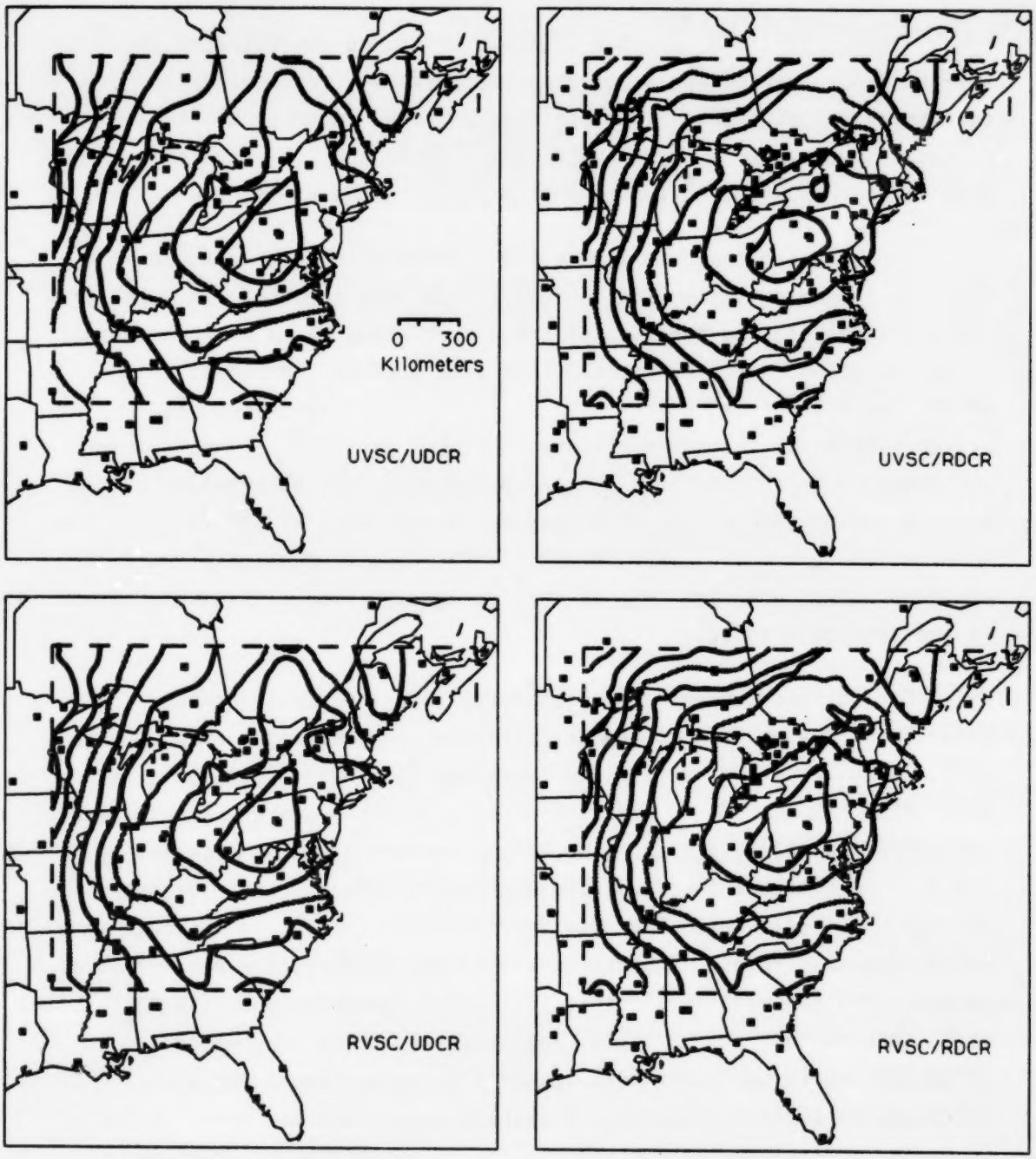

FIGURE 5.4. Contours of pH Estimates of the Four Subsets Using the UDDC or Relaxed Valid Sample Criteria (UVSC or RVSC) and the UDDC or Relaxed Data Completeness Rating (UDCR or RDCR). The Values of the Contour Lines are Given in Figure 5.1.

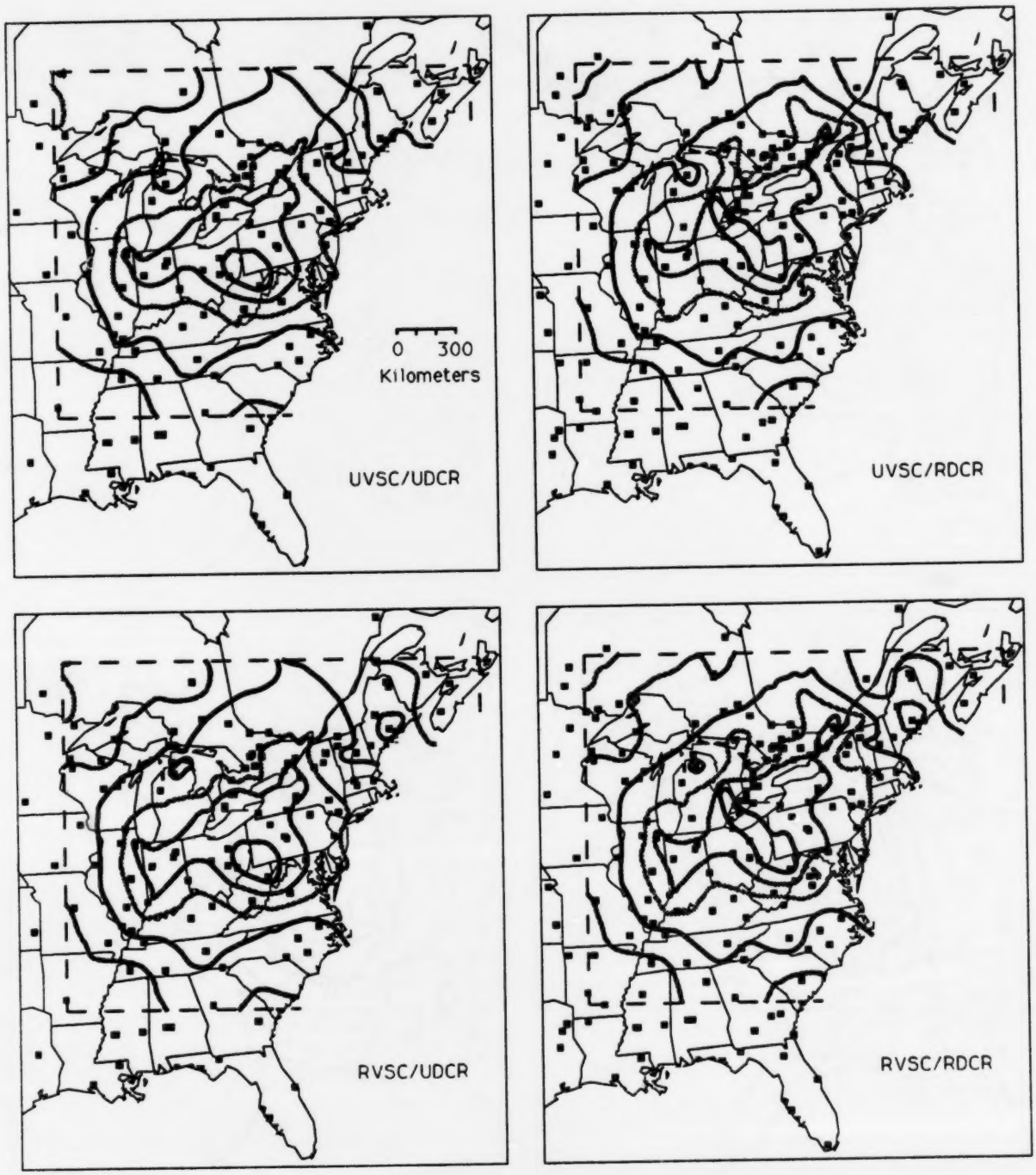

FIGURE 5.5. Contours of Sulfate Concentration (mg/l) Estimates of the Four Subsets Using the UDDC or Relaxed Valid Sample Criteria (UVSC or RVSC) and the UDDC or Relaxed Data Completeness Rating (UDCR or RDCR). The Values of the Contour Lines are Given in Figure 5.2.

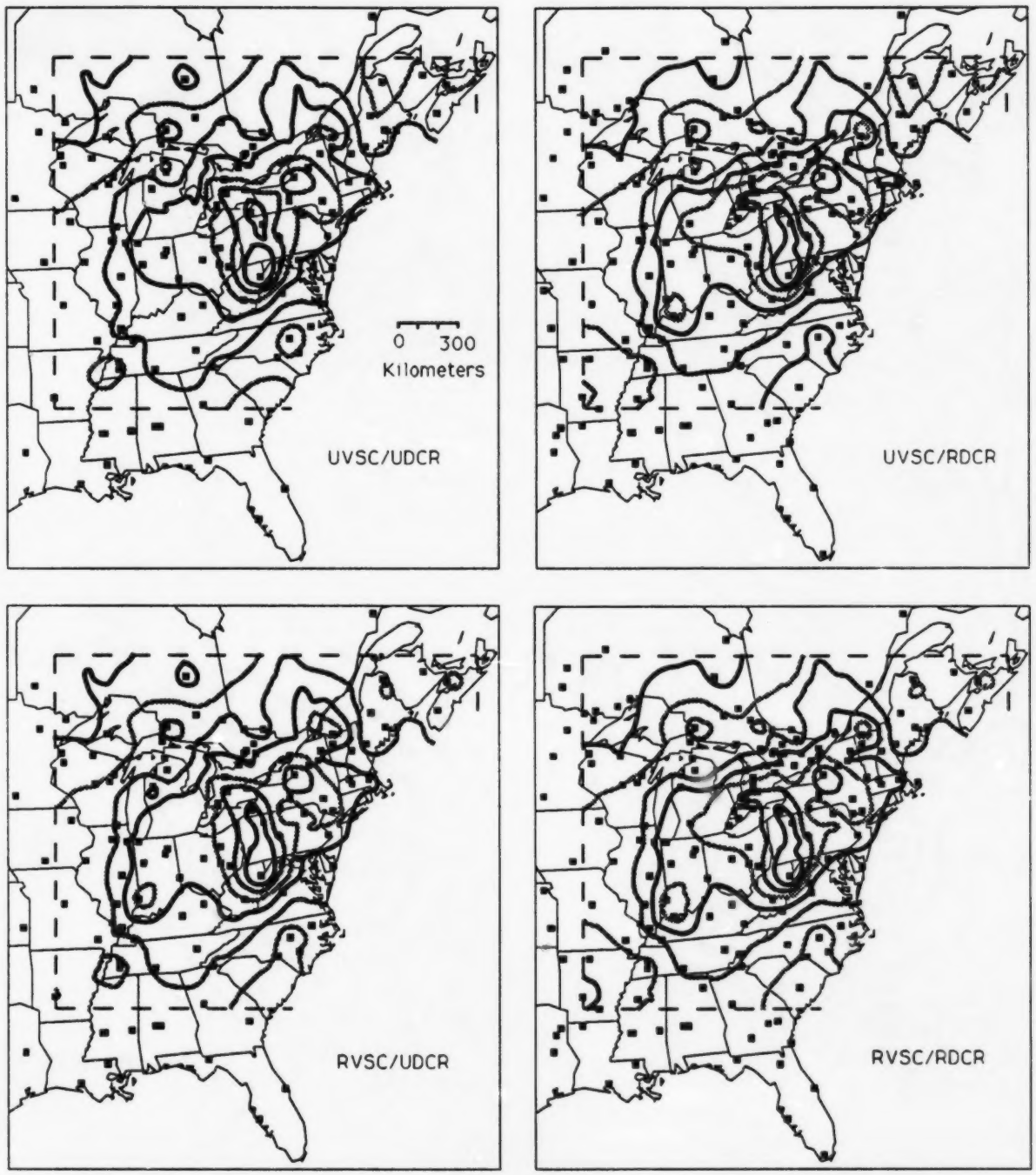

FIGURE 5.6. Contours of Sulfate Deposition (g/sq m) Estimates of the Four Subsets Using the UDDC or Relaxed Valid Sample Criteria (UVSC or RVSC) and the UDDC or Relaxed Data Completeness Rating (UDCR or RDCR). The Values of the Contour Lines are Given in Figure 5.3.

The sulfate deposition estimates (see Figure 5.6) increase in southern Ontario, southern Wisconsin and northern Ohio when the number of sites used increase, from UDCR to RDCR. The 3.0 g/m^2 contour moved approximately 300 kilometers west. The presence of two sites on the southwestern border of Indiana bordering on Illinois (ADS ID 420a; NADP; Vincennes, Indiana) and bordering on Kentucky (ADS ID 154a; UAPSP; Rockport, Indiana) caused the 2.5 g/m2 contour to move approximately 250 kilometers south and an area with a diameter of over 100 kilometers to have depositions greater than 3.0 g/m^2. The increased number of sites also caused decreases in Quebec, Arkansas, northern Mississippi and northern Alabama. The change in the values of the observations . UVSC versus RVSC, has the effect of further increasing the deposition in southwestern Indiana and decreasing the deposition in Maine and New Brunswick.

Figure 5.7 shows the effect of the Parsons, West Virginia site (ADS ID 075a; NADP). The top shows the sulfate concentration and the bottom shows the sulfate deposition, the left side has the contours using the UVSC/UDCR subset while the right side has the contours using the same subset of observations less Parsons, West Virginia. As seen in this figure, the removal of this one unusual site causes reductions in both the concentration and deposition estimates in a five state region (Ohio, Pennsylvania, Maryland, Virginia and West Virginia).

5.2 CONTOUR MAPS OF THE DIFFERENCES

Figures 5.8, 5.9, and 5.10 show the contoured differences for selected subsets of pH, sulfate concentration and sulfate deposition, respectively. The upper left map is the difference between the UVSC/UDCR and the RVSC/RDCR subsets. This figure demonstrates the magnitude and extent of the effects of going from the UDDC to the relaxed definitions of both the valid sample criteria and the data completeness ratings. The upper right map is the difference between the UVSC/UDCR and the UVSC/RDCR subsets. The difference in these groups are the additional sites, the values at the sites do not change. The lower left map is the difference between the UVSC/UDCR and the RVSC/UDCR

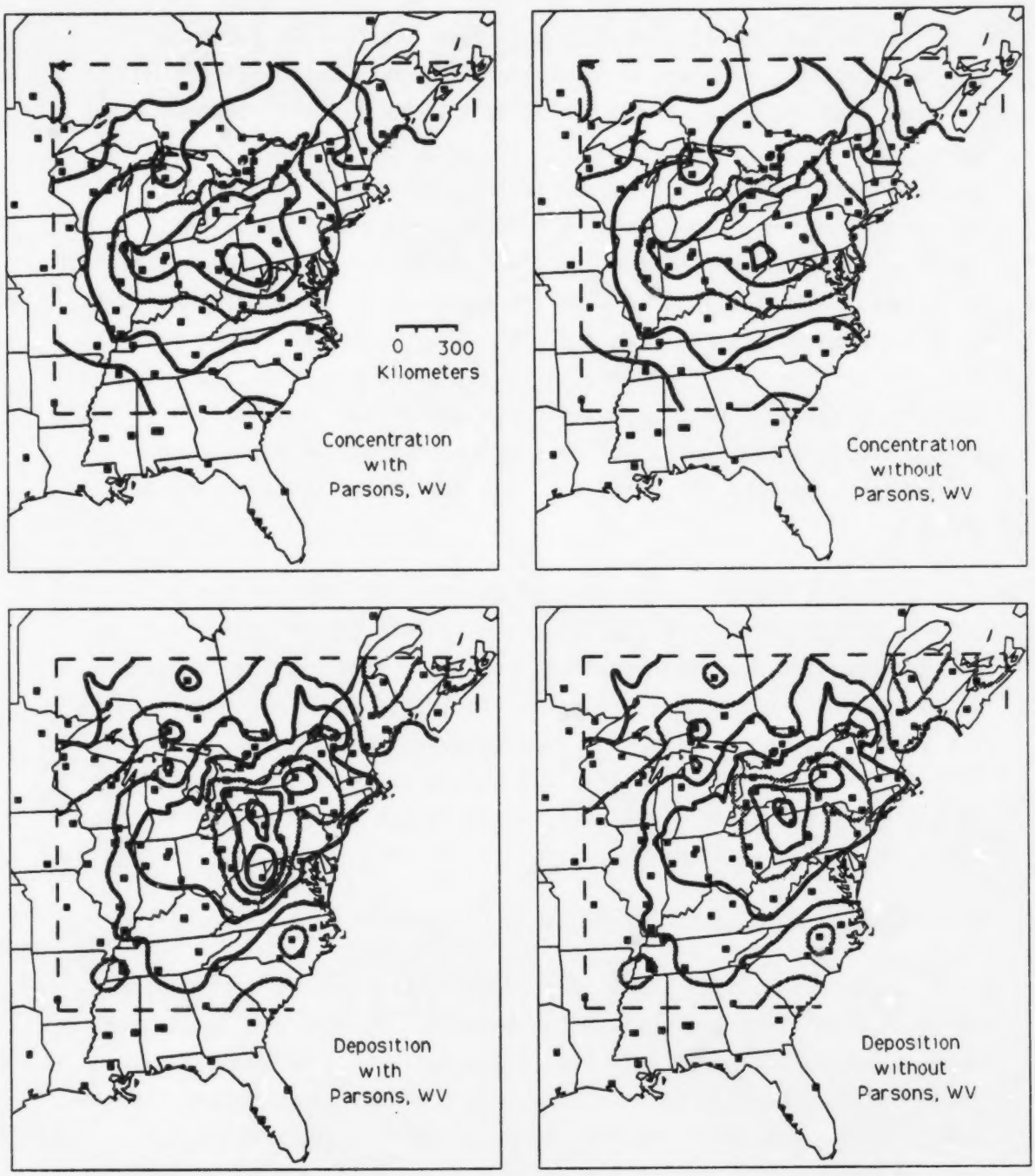

FIGURE 5.7. Comparison of Sulfate Concentration and Deposition Estimates With and Without Parsons, West Virginia Site Present. The Rest of the Sites Belong to UVSC/UDCR Subset. See Figures 5.2 and 5.3 for the Values of the Contour Lines.

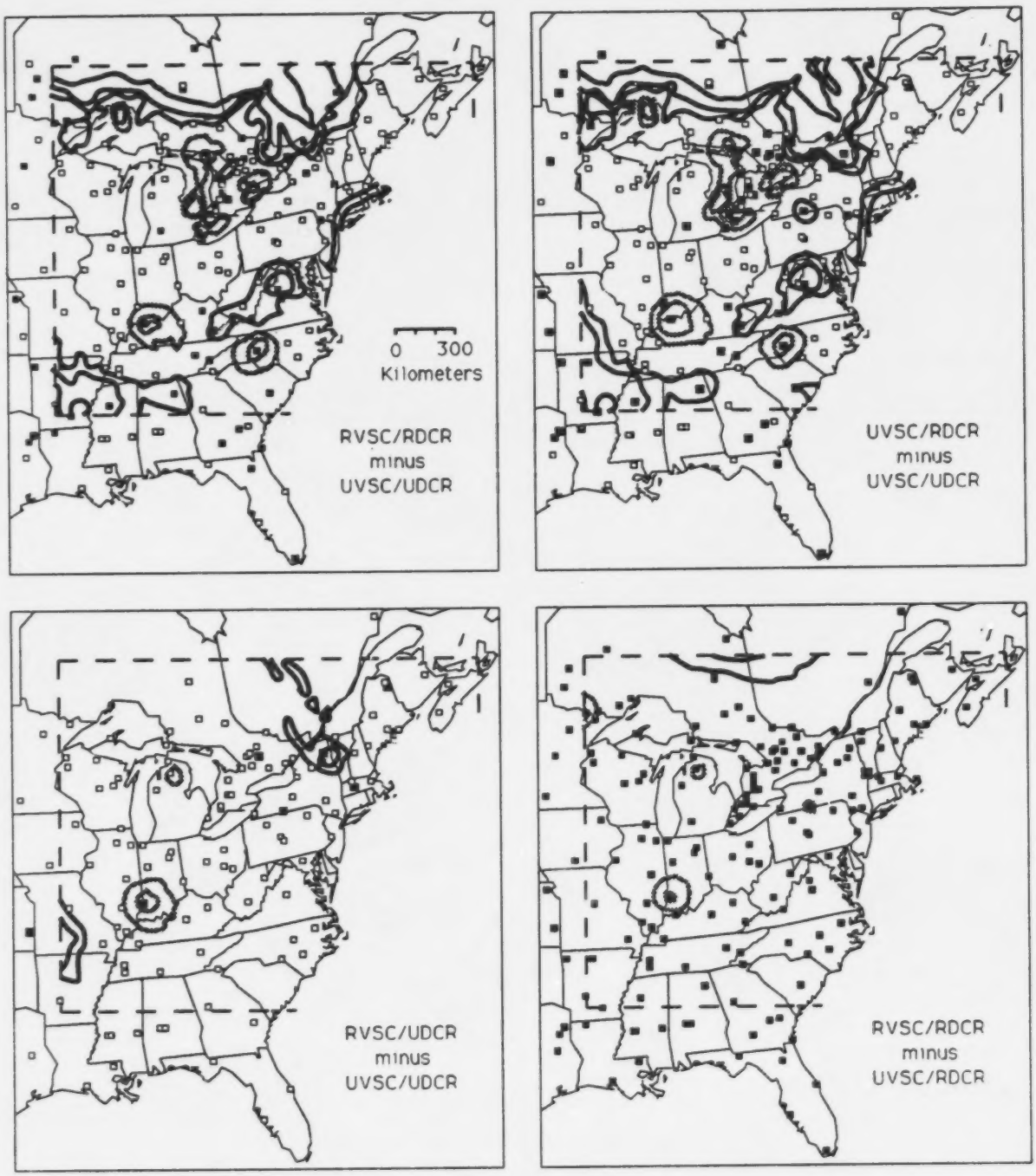

Figure 5.8. Differences in pH estimates for selected pairs of subsets. The dark lines indicate an increase in the estimate and the light lines indicate a decrease in the estimate. The outer contour is 0.025, the middle contour is 0.05 and the interior contour is 0.10.

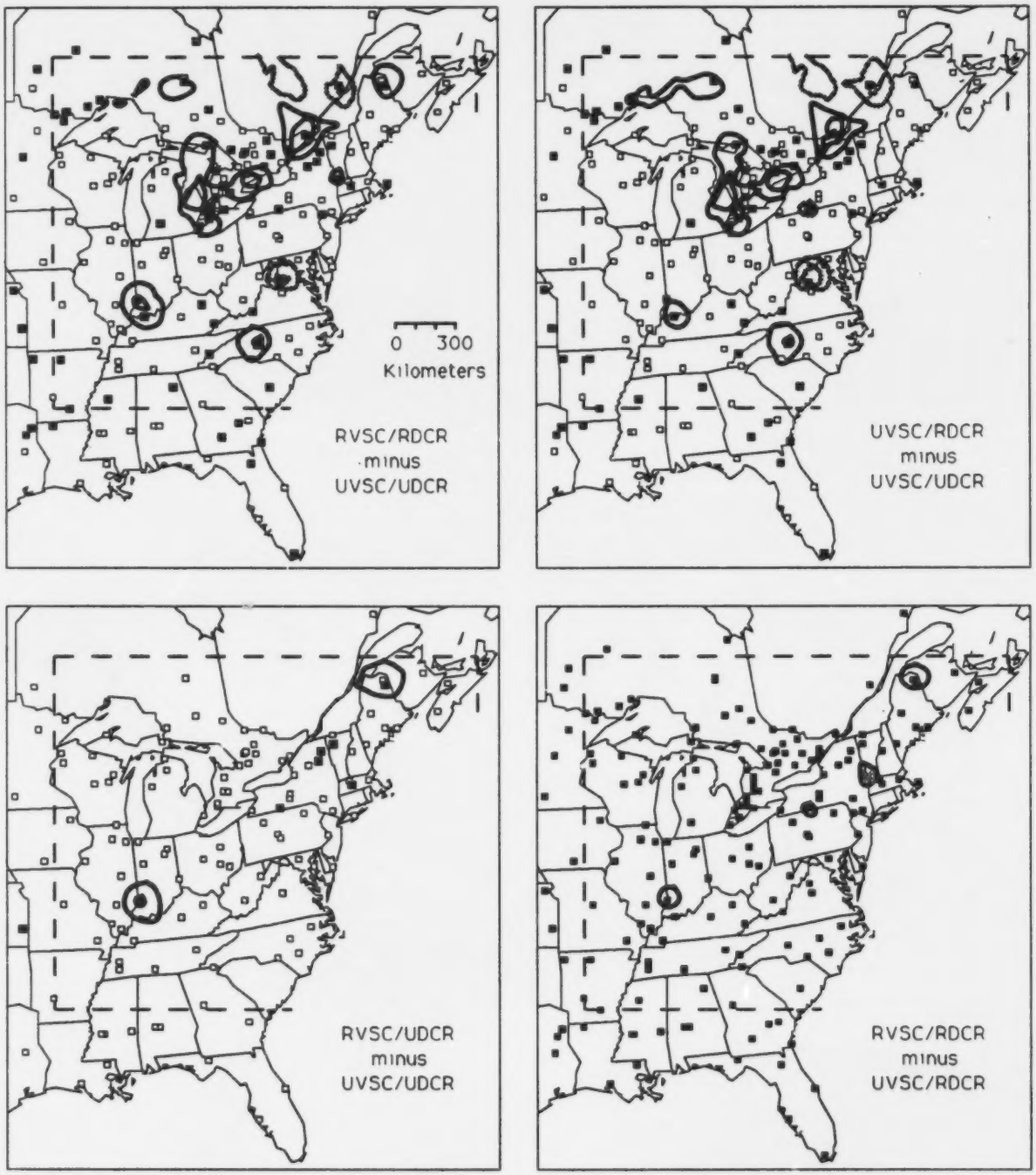

FIGURE 5.9. Differences in Sulfate Concentration Estimates for Selected Pairs of Subsets. The Dark Lines Indicate an Increase in the Estimate and the Light Lines Indicate a Decrease in the Estimate. The Outer Contour is 0.25 mg/l and the Interior Contour is 0.5 mg/l.

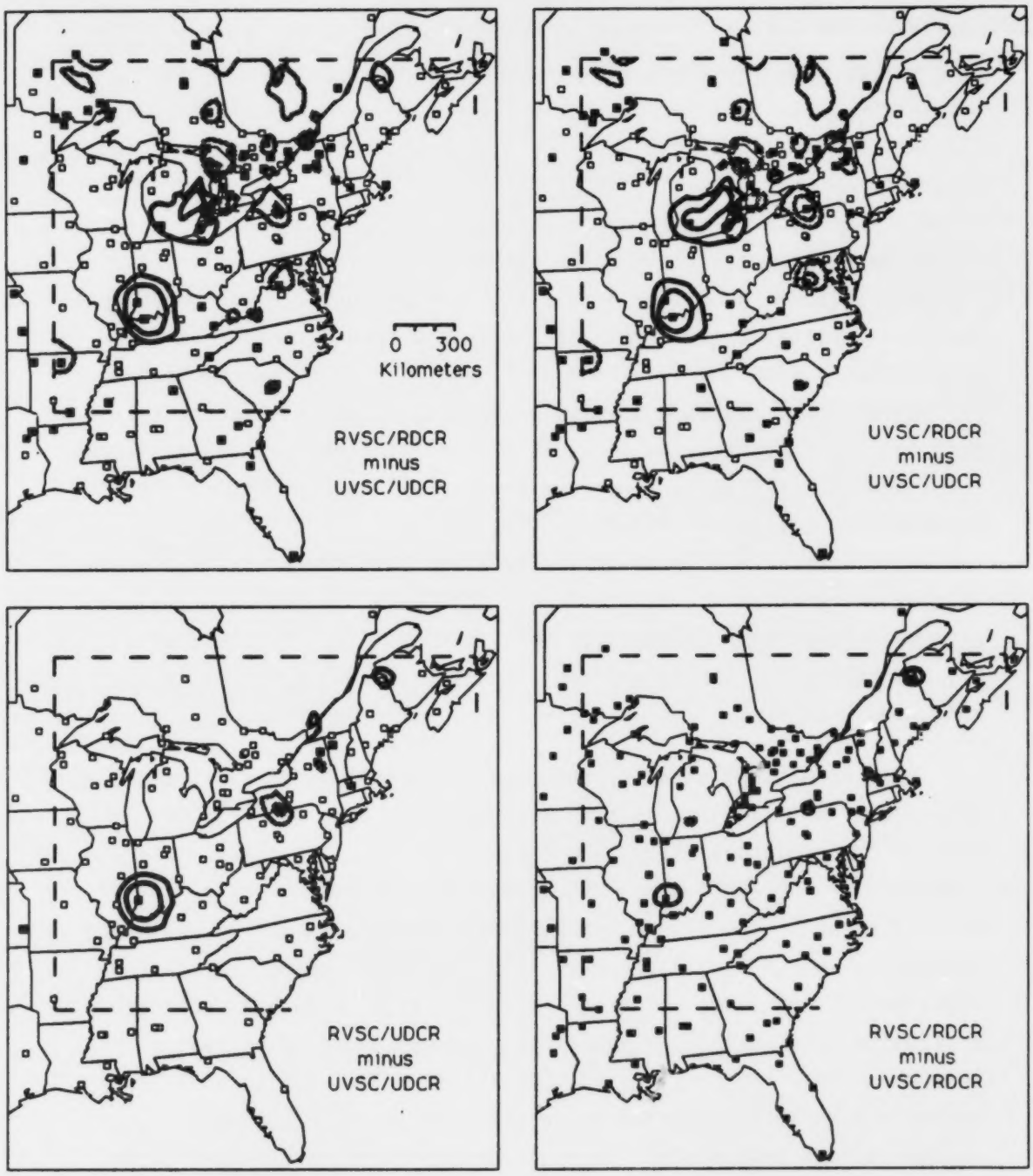

FIGURE 5.10. Differences in Sulfate Deposition for Selected Pairs of Subsets. The Dark Lines Indicate an Increase in the Estimate and the Light Lines Indicate a Decrease in the Estimate. The Outer Contour is 0.25 g/sq m and the Interior Contour is 0.5 g/sq m.

subsets. The primary difference in these groups is the change in the site values, however there are a few additional sites. The lower right map is the difference between the UVSC/RDCR and the RVSC/RDCR subsets. The differences in these groups are the changes in the values of the observations with only one additional site on the Vermont-New York border. For each of these maps, the dark contours indicate an increase in estimates from the the UDDC to the relaxed definition(s) while the lighter contours indicate a decrease in the estimates. For pH the outer contour indicates a difference of 0.025, the second contour is for a difference of 0.05 and the third contour is for a difference of 0.1. For sulfate only two contour levels are used. The outer contour is 0.25 mg/l for the concentration and 0.25 g/m^2 for the deposition, while the inner contour is 0.50 mg/l for the concentration and 0.50 g/m^2 for the deposition. The additional sites that are used in each comparison are indicated with dark squares while the site locations that are the same (although the value of the observation may have changed) are indicated with white squares. In the maps showing the differences between strict-all and relaxed-all, only one additional site is used and it is indicated with an X.

The effects of changing the subsets for pH, shown in Figure 5.8, extend over a large area in many different regions. As seen in this figure, the additional sites are the primary cause of these differences (the maps of RVSC/RDCR minus UVSC/UDCR and UVSC/RDCR minus UVSC/UDCR are quite similar). The few additional sites in Ontario and Quebec cause an area whose length is greater than 1000 kilometers to be increased by more than 0.1 pH units. The additional sites in Arkansas, northern Mississippi and northern Alabama also increases the pH estimates throughout this region as much as 0.1 units. The additional sites in southern Ontario reduced the pH in this region, although much of this region is over Lake Huron. Several additional sites effected 'local' regions of over one hundred kilometers in diameter, with several of the regions have considerable area with estimates that changed by more that 0.05 units. Only the five sites with the largest changes in their pH observations (see Table 2.6, sites 047a (Jasper, New York), 208a (Lac Le

Croix, Ontario), 241a (Gaylord, Michigan), 420a (Vincennes, Indiana), and 495a (Mooseonee, Ontario)) have a noticeable effect (see RVSC/RDCR minus UVSC/RDCR). Of these sites, 495a (Mooseonee, Ontario) which is the northern most site shown in Ontario has the largest effect. The size of this effect is due to the sparsity of data in the region. As seen in Table 2.7, the changes in the values for sites 420a (Vincennes, Indiana) and 495a (Mooseonee, Ontario) are primarily due to one sample with extremely unusual pHs. These samples have extremely poor collection efficiencies (2.9% and 2.0%, respectively, of the sample volume predicted from the rain gauge is actually present in the collector). Site 047a (Jasper, New York) is very unusual, on one map it causes an increase, on another map it causes a decrease and on the other two maps it has no effect. This site has only one sample that is added (see Table 2.7), however, it is also the only sample in June that is analyzed, thus when the sample is removed, all of June is essentially removed. Without this sample, the pH value is large compared to it's neighboring sites. When the sample is added, the pH decreased and the site is no longer large compared to it's neighboring sites.

The effects of changing the subsets for sulfate concentration, shown in Figure 5.9, are greatest in southern Ontario. As seen in this figure, the additional sites are the primary cause of these differences. Most of the new sites are in southern Ontario and have higher concentrations than their neighboring sites. These sites have poor UDDC data completeness ratings and are only included when the data completeness rating in relaxed. Their poor ratings are primarily because of their low collection efficiencies. The three sites with the largest changes in the sulfate concentrations (see Table 2.4, sites 047a (Jasper, New York), 163a (Caribou, Maine) and 420a (Vincennes, Indiana)) have a noticeable effect. The extent of the effects are related to the density of neighboring sites, with the size increasing as the density decreases. The extent of the effect due to site 163a (Caribou, Maine), is effected by site 436a (Presque Isle, Maine) that is just southwest of it. When the UDDC valid sample criteria is used to select the samples, these two sites are similar (1.32 mg/l at 163a verses 1.55 mg/l at 436a), thus there is no effect on the UVSC/RDCR minus UVSC/UDCR map.

When the relaxed valid sample criteria is used to select the samples, both site's observations increase (1.84 mg/l at 163a verses 1.70 mg/l at 436a), thus the extent of the effect shown on the has a RVSC/RDCR minus UVSC/RDCR map has a diameter of a little over 100 kilometers (the averages of these two sites change from 1.44 mg/l to 1.77 mg/l). However on the RVSC/UDCR minus UVSC/UDCR map the diameter of the area effected has increased to over 200 kilometers because the values change from 1.32 mg/l (163a only) to 1.77 mg/l. The increase in the sulfate concentration at site 163a is due to two samples with unusually high sulfate concentration (52 mg/l precipitation weighted average) with very low collection efficiencies (11.2% and 24.8%). Sites 420a along the the Indiana-Illinois border (Vincennes, Indiana) and 154a along the Indiana-Kentucky border (Rockport, Indiana) also effect each other. Under the strict criteria for selecting samples their sulfate concentrations are 2.62 mg/l and 2.65 mg/l, respectively. However only site 154a has an effect when UVSC/RDCR and UVSC/UDCR are compared because of the lower observations to the south of 154a. However when the valid sample criteria is relaxed, site 420a increases to 3.08 mg/l and causes an effect with a diameter of close to 200 kilometers without the present of 154a and about 100 kilometers when 154a is present. The large increase at site 420a is primarily due to one sample with a concentration of 69 mg/l and a collection efficiency of only 2.9%. Finally, as with pH, the effects of site 047a (jasper, New York) change with the different maps and the reasons are the same as before.

The effects of changing the subsets for sulfate deposition, shown in Figure 5.10, are also greatest in southern Ontario. As seen in this figure, the additional sites are again the primary cause of these differences. Unlike the sulfate concentration, not all the effects, in southern Ontario, are an increase in the estimates. While the sulfate concentration (see Figure 5.9) at some sites are high compared to the neighboring sites, their sulfate deposition is low when compared to the same neighboring sites. This anomaly is a result of the very low precipitation at these sites. The effects of sites 154a and 420a in southwestern Indiana are larger than those shown for the sulfate concentration primarily because of the high precipitation at site 154a.

These sites together account for an increase of 0.5 g/m^2 in sulfate deposition over an area with a diameter of over 200 kilometers. As with pH and sulfate concentration, site 047a remains a very unusual site. Although the sulfate concentration increases to a level that is similar to it's neighboring sites, when the valid sample criteria is relaxed, this site has a low precipitation amount as compared to its neighbors. Thus, although the sulfate deposition increase when the valid sample criteria is relaxed, this new value is still low compared to it's neighboring sites.

The extent and magnitude of effect that the Parsons, West Virginia site has on the 'local' sulfate concentration and deposition estimates are shown in Figure 5.11. The extent of this effect is over a region with a diameter of approximately 400 kilometers. This region is limited by the use of only the eight closest sites in the estimation process. The magnitude of the effect increases to over 0.5 mg/l for the concentration and 1.5 g/m^2 for the deposition. The region of those magnitude's of effect or approximately 100 kilometers. The magnitude of the effect of the sulfate deposition is much greater than that for the sulfate concentration because of the high precipitation at this site.

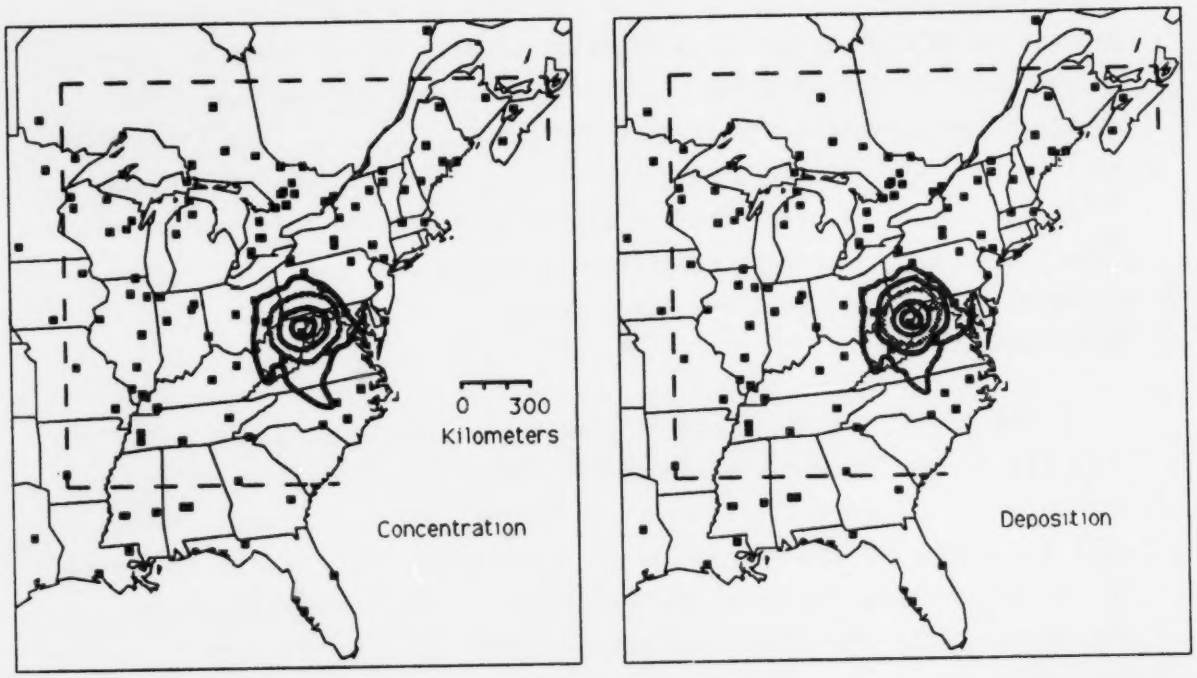

FIGURE 5.11. Extent and Magnitude of Effect the Parsons, West Virginia Site has on the Sulfate Concentration and Deposition. The Concentration Contours are 0.5, 0.25, 0.10 and 0.001 mg/l and the Deposition Contours are 1.5, 1.0, 0.5 0.25 and 0.001 g/sq m.

6.0 CONCLUSIONS

Application of UDDC valid sample criteria requires that the UDDC rating be used to ensure representativeness throughout all seasons. This is a conservative position for inclusion of data for maps. As seen with site C47a and other sites shown in Table 2.7, when the UDDC valid sample criteria is used, blocks of data over a period of greater than a month may be lost. When a site has seasonal trends, the loss of that much data can adversely effect the annual estimates.

Relaxed valid sample criteria may or may not lead to representative annual summaries for the year. Sites must be evaluated with respect to other nearby sites or years. Seasonal criteria may not guarantee representativeness. That is, using the UDDC data completeness rating requirement does not protect you. As seen in Table 2.7, at a number of sites, the relaxed valid sample criteria let a number of extremely unusual samples to be included in the annual estimates. However, all these samples have very small collection efficiencies. Possibly, the collection efficiency needs to be examined on a sample by sample basis, instead of seasonally and annually.

Representativeness of a site for its surrounding area is very important with a sparse network. Does the sulfate concentration and deposition at the Parsons, West Virginia site represent the area within 200 kilometers of it?

Although the relaxed data completeness rating allows the number of sites used to increase by over 50%, except for a few sites, these additional sites did not change the spatial patterns of wet deposition on a region scale. Most of the changes due to the additional sites are on a local scale where these differences are smaller than the scale used in regional isopleth maps. The few additional sites which do have a profound effect are located in areas where there is a sparsity of sites (e.g. northern Ontario) or whose summaries are changed markedly due to either the addition of an extremely unusual sample or the addition of a large contiguous number of samples. Thus, for contour maps whose

objective is to show regional pattern, the key issue is not the number of sites but the location of the site and the validity of the samples from the site.

There are two sources of uncertainty in the contour maps that need to be addressed. First, the within-site variation in the annual summaries. Because there are so few collocated sites, the within-site variation is poorly estimated and thus any variance estimate from kriging is also poorly estimated. Second, the variation from year to year in the annual summaries at a site have not been considered. For example, at Parsons, West Virginia the annual sulfate depositions (g/m^2) are 4.4 (1979), 4.4 (1980), 4.6 (1981), 4.0 (1982), 3.1 (1983), 3.4 (1984), 4.8 (1985), 5.3 (1986) and 3.0 (1987). It should be noted that in 1985 and 1986, 19% and 9%, respectively, of the precipitation has no chemistry results for sulfate. This occurs primarily in months when the sulfate concentration is low at this site (late fall). Additionally, in 1987 the annual precipitation was only 73% of the average annual precipitation for the previous eight years.

For network operations, the implication of this study is that sites must give valid data for the entire year. The loss of a large number of contiguous samples renders the site useless for the purpose of annual summaries. The relationship between small sample collection efficiency and the representativeness of the sample's chemistry needs to be reevaluated.

For network design, the implication of this study is that the total number of sites is less important than the representativeness of the site. When considering a region the size of the eastern United States, where the sheer magnitude of the region forces sites to be hundreds of kilometers apart, the summaries from one site can profoundly impact a large region. If that site is not representative of the region between sites, then it will bias the results.

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APPENDIX A

COMPARISON OF 1985 pH CONTOUR MAPS

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June 22, 1988

This paper gives a comparison of the 1985 pH maps that appear in the NAPAP Interim Assessment (NAPAP 1987) and in the NADP 1985 Annual Data Summary report (NADP 1987).

Figure 1 reproduces the NADP report map and Figure 2 reproduces the NAPAP report contour map, prepared by Pacific Northwest Laboratory (PNL). The first feature of the maps that differs is the use of different contour levels. This makes any comparison difficult. Judgement of whether the maps agree depends on who makes the judgement and what is the intended purpose of the maps. An appropriate purpose for the map appears to be a semi-quantitative display of the spatial pattern of pH during 1985. With this as the purpose, the two maps appear to agree.

The production of contour maps is a problem of surface estimation and display. All solutions will not agree exactly in the location of contour lines but strong qualitative agreement should be expected. I have taken a closer look at the production process for the maps. First, I reviewed the production processes used by NADP and PNL to determine the steps used. Second, I requested that PNL and NADP prepare several alternative maps to investigate possible reasons for quantitative differences in the maps.

PRODUCTION PROCESSES

The production of a contour map includes the following:

- Calculation of an annual pH value at a site,
- Selection of sites to be used in surface estimation,
- Selection of a surface estimate technique,
- Display of the estimated surface,
- Production of final document quality contour map.

NADP and PNL use the same calculation procedure to obtain an annual pH value for a site. The pH values for sites that NADP and PNL both used in preparing

APPENDIX A

COMPARISON OF 1985 pH CONTOUR MAPS

the maps agree in all cases. Both use pH to the nearest hundredth in the production process. Note that pH values that appear on the maps are rounded to the nearest tenth. Because of the rounding, contour lines may include or exclude sites that appear to be on the "wrong" side.

The NADP and PNL maps do use different sites for the surface estimation. NADP uses only NADP/NTN network sites. NADP used 123 NADP/NTN sites and PNL used 183 sites from multiple networks. PNL uses sites from the NADP/NTN, UAPSP, MAP3S, CAPMoN, and APIOS networks. Fewer NADP sites (20) are used by PNL than by NADP. This is due to using different criteria for inclusion of a site. The major difference is that PNL includes a quarterly criteria as well as an annual criteria. The underlying data completeness measures are calculated the same, the difference is in which measures are applied and what cutoff criteria is used. Based on our current knowledge on the relationship between the criteria and the "representativeness" of the annual summary, I do not believe that a case can be made for preferring either the NADP or the PNL criteria. Both are reasonable choices.

NADP and PNL use entirely different surface estimation algorithms. The initial step in both algorithms is to estimate the surface on a regular grid. The regular grid is then used to determine the location of the contour lines. NADP uses a grid on a transverse mercator projection at an unknown but reasonable grid density. PNL uses an 80 km grid on a Lambert conic projection that is near-distance preserving. NADP uses the SURFACE II graphics system (Sampson 1984). The gridding routine uses a constrained distance-squared weighting function applied to the eight nearest site locations (a maximum search radius is imposed). PNL uses the kriging algorithms in BLUEPACK software (Delfiner 1979). Kriging also is distance-weighted but the distance weights are derived from the variation observed in the site data. The pH weights are from a spherical semi-variogram. Eight sites are used with a restriction that each octant from the grid node contributes a site, if available within a maximum search radius.

Smooth contour lines are interpolated from the regular grid. NADP uses the "CONT" function in Surface II, which uses a piecewise Bessel interpolation within a grid cell. PNL uses the DISSPLA graphics contouring function with a cubic spline interpolation, termed "spline under tension." I review the maps that are computer generated for consistency with the monitoring site data. This review typically includes removing contours in the West, deleting extensions of contours over the ocean, and subjectively smoothing contours, especially in data sparse regions, to remove non-data supported features.

ALTERNATIVE MAP COMPARISON

Since NADP and PNL used different sets of sites and different surface estimation and contouring algorithms, four alternative maps are produced for the four possible combinations. As a point of departure, Figures 1 and 2 are the original maps as they appeared in the NAPAP interim assessment and the NADP 1985 Annual Data Summary. The sites included in the NADP data set (123 sites) and the PNL data set (183 sites) are shown in Figures 3 and 4, respectively.

For the comparison, PNL produced two maps (Figures 5 and 6) using our standard surface estimation and contouring procedure. Contour levels were changed to be the same as the NADP original map. The same kriging semi-variogram is used for both maps (same as used in NAPAP map). The maps provide an assessment of differences that arise from using different subsets of sites. My assessment is that the maps agree very well east of the Mississippi River within the United States. The 4.7 and 4.9 contours have bends in the south that are not supported by site data. These would be subjectively smoothed to remove "artificial" features. The 5.1 contour extends into the West where contouring is questionable. The 4.5 contour differs in Canada and Maine due to the PNL data set including Canadian sites. The 4.3 contour differs in northern New York. Other differences in the contours are small. In Figure 7, an expanded view of eastern North America for the original PNL NAPAP map is given for comparison.

NADP used the NADP contouring algorithm to produce a map based on the NADP data set sites (Figure 8) and the PNL data set sites (Figure 9). The maps agree very well east of the Mississippi within the United States. The differences between them are similar to those present between the two PNL maps. The areas, west of Mississippi and Canada, where the density of sites differs between the two data sets show the greatest differences.

The NADP map (Figure 8) and the PNL map (Figure 5) using the 123 sites in the NADP data set are remarkably similar. The north, northeast and southwest portion of the NADP 4.3 contour extends farther than the PNL contour. The southern portion of the 4.7 NADP contour extends into Texas while the PNL contour does not. Larger differences occur for the 5.1 contour in the west, reflecting sparse data support in this region. The NADP map (Figure 9) and the PNL map (Figure 6) using the 183 sites in the PNL data set show differences remarkably similar to the previous comparison.

SUMMARY

My assessment of the comparison of the different data sets and the different "contouring" algorithms used by NADP and PNL is that they produce remarkably similar maps. Agreement is best where the density of sites is greatest and poorest where the density is lowest. Inclusion of Canadian sites does aid in completing contours in the northeast. This is to be expected. When the algorithms are compared on the same data set, the differences are no greater than differences observed when using same algorithm with different data sets. The computer drawn NADP maps appear to be smoother than the computer drawn PNL maps. This is related to the density of grids used and the selection of a smoothing parameter.

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FIGURE 1. NADP Original 1985 Annual Data Summary pH Map

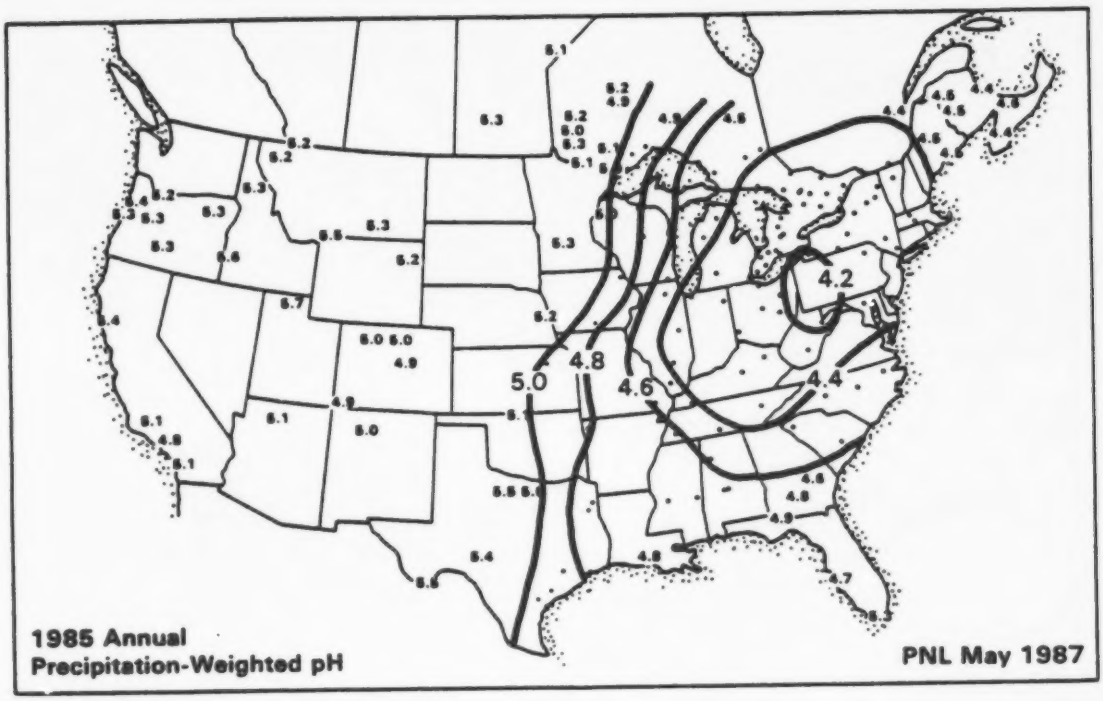

FIGURE 2. PNL Original NAPAP Interim Assessment Document 1985 pH Map

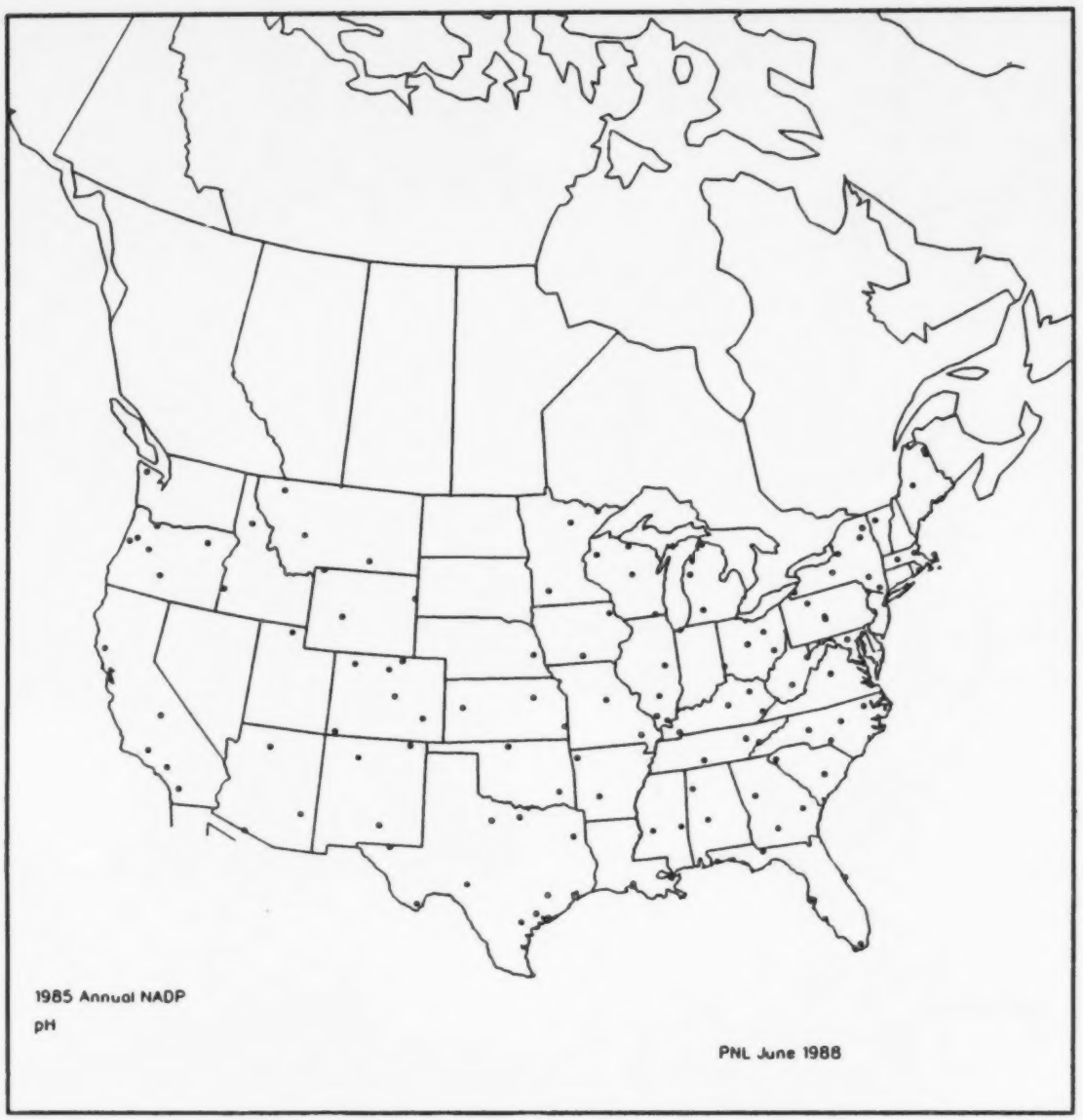

FIGURE 3. Sites Used in NADP pH Data Set

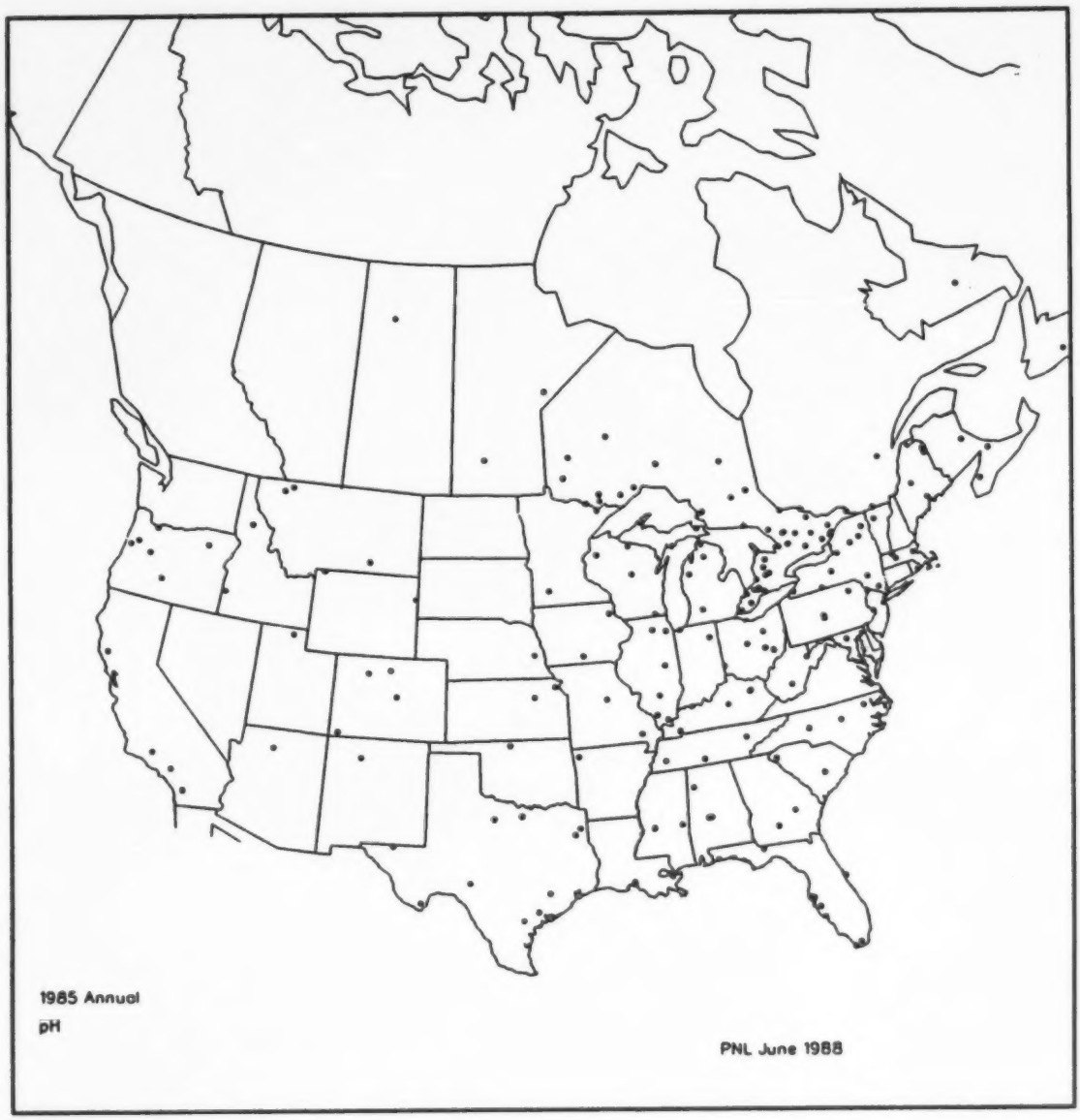

FIGURE 4. Sites Used in PNL pH Data Set

FIGURE 5. PNL Kriging Map Using NADP Data Set Sites

FIGURE 6. PNL Kriging Map Using PNL Data Set Sites

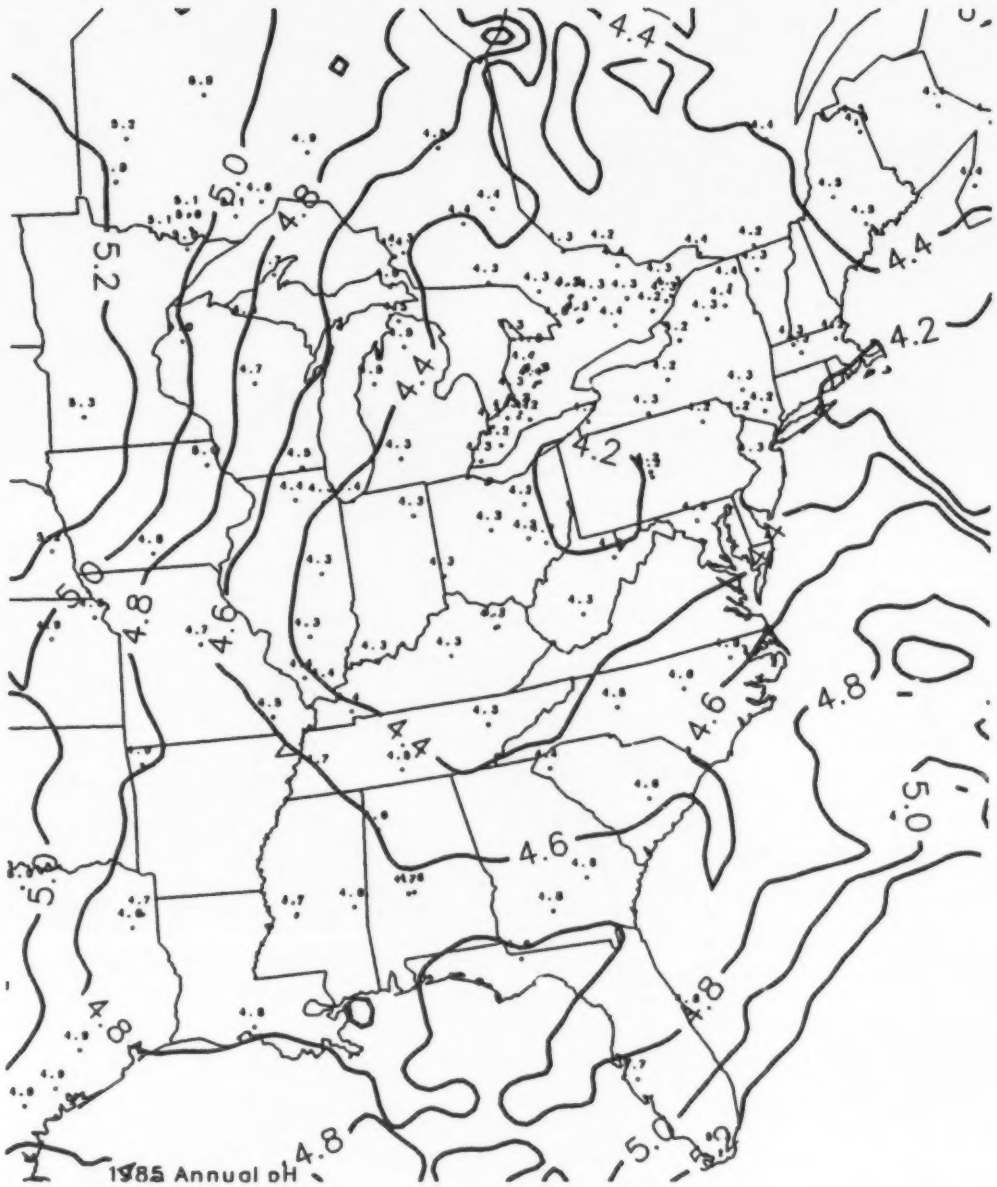

FIGURE 7. PNL Computer Drawn Map for Original NAPAP Interim Assessment pH Map

FIGURE 8. NADP Map Using NADP Data Set Sites

FIGURE 9. NADP Map Using PNL Data Set Sites

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